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INNOVATIONS IN MATERIALS DESIGN, PART I: THE DESIGN OF INORGANIC COMPOUNDS PART II: SEARCHING FOR NEW ELECTRO-OPTICAL, FERRO-ELECTRIC, SUPERCONDUCTING, AND SEMI-CONDUCTING MATERIALS

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This technical report has been reviewed and is approved for publication.

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The use of computer learning strategies for predicting inorganic compounds which are believed promising as new electro-optical, ferro-electric, superconducting or semiconducting materials is explained. Prediction reliability utilizing these computer learning strategies is based on: 1) expert selection of example compounds, 2) expert assessment of data for computer learning, and 3) comparison of predictions which have been obtained using various feature sets. The classes of the inorganic compounds most promising for searching for new electro-optical, ferro-electric, superconducting, and semiconducting materials are directly based on the analysis of the application domains and the known data. The results of predicting the crystal structure types at normal pressure and room temperature for the compound with composition of AB2Se4 are presented. Types considered were chalcopyrite, Th3P4, CaFe2O4, Yb3S4, Yb3Se4, PbGa2Se4, NiCr2Se4, spinel, or olivine. Analysis of predictions showed that the structures resembling olivine and NiCr2Se4 are an inherent feature of the compounds with composition A(IV)B(II)2Se4, but the structure types Th3P4 and NiCr2Se4 are characteristic of compounds with composition A(II)B(III)2Se4. Prediction of the crystal structure types at standard conditions for compounds with composition ABX2 were also carried out. Types considered included chalcopyrite, a or b-NaFeO2, a-LiFeO2, or TlSe.

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The Design of Inorganic Compounds:
Searching for new electro-optical, ferro-electric, superconducting and semiconducting materials

February 1995

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Abstract

The use of computer learning strategies for predicting inorganic compounds which are believed promising as new electro-optical, ferro-electric, superconducting or semiconducting materials is explained. Prediction reliability utilizing these computer learning strategies is based on: 1) expert selection of example compounds, 2) expert assessment of data for computer learning, and 3) comparison of predictions which have been obtained using various feature sets. The classes of the inorganic compounds most promising for searching for new electro-optical, ferro-electric, superconducting, and semiconducting materials are directly based on the analysis of the application domains and the known data. The results of predicting the crystal structure types at normal pressure and room temperature for the compound with composition of AB_2Se_4 are presented. Types considered were chalcopyrite, Th_3P_4, $CaFe_2O_4$, Yb_3S_4, Yb_3Se_4, $PbGa_2Se_4$, $NiCr_2Se_4$, spinel, or olivine. Analysis of predictions showed that the structures resembling olivine and $NiCr_2Se_4$ are an inherent feature of the compounds with composition $A(IV)B(II)_2Se_4$, but the structure types Th_3P_4 and $NiCr_2Se_4$ are characteristic of compounds with composition $A(II)B(III)_2Se_4$. Prediction of the crystal structure types at standard conditions for compounds with composition ABX_2 were also carried out. Types considered included chalcopyrite, α or β -$NaFeO_2$, α-$LiFeO_2$, or TlSe.

Subject Terms (Key Words)

Concept formation, computer learning, prediction, inorganic compound, electro-optical, ferro-electric, superconductor, semiconductor, chalcopyrite, spinel.

Foreword

This report was prepared by the above identified research team under EOARD Special Contract SPC-94-4097. This is an interim report summarizing research carried out over a period of six months from September 1994 to February 1995. This work was carried-out in close contact with researchers of the Materials Directorate, Wright Laboratory. We appreciate the management leadership of Dr. Steven R. LeClair. We thank Drs. Steven R. LeClair and Allen G. Jackson for their assistance.

[Added text by A. G. Jackson and S. R. LeClair:

This contract program represents a collaboration between Dr. Kiselyova's group at the Baikov Institute in Moscow, Russia and the Materials Process Design Branch of the Materials Directorate, Wright Laboratory.

The general field of study may be best described as the 'crystal engineering of new materials'. As opposed to an *ab initio* approach to materials design, this field utilizes pattern recognition methods applied to empirical data to synthesize new knowledge about materials at the atomic level.

Current research in the Materials Process Design Branch is concerned with self-directed control of processes and automation of materials design and discovery. Of the many computational strategies available to approach this problem, several new methods have been the focus of attention. These include rough sets and pyramidal nets. Rough sets is of interest because of its ability to classify quantitative and qualitative data and produce rules based upon classifications of data. The method used by the authors of this report, referred to as pyramidal nets, is attractive because of its ability to provide a logical expression of the classification of complex objects and to create new objects (concepts) from the originals automatically. Comparative prediction of properties of materials using these and other methods needs to be examined and is the purpose of our longer term research interests.

This report presents results from a heretofore unavailable source, the Former Soviet Union, as applied to the problem of the design of new materials using the pyramidal net approach. It illustrates several problems associated with the prediction of properties while providing the reader with an appreciation of the potential for these methods in the design of new materials.

It also must be noted that we have revised some of the followning text in the origianl report from Dr Kiselyova's group in order to clarify the meaning of some of the contents.

We also acknowledge the support provided by Dr. Osama Elbayoumi, of the European Office of AFOSR, for enabling the interaction between ourselves and Dr. Kiselyova's group.]

1. INTRODUCTION

The project's goal is to develop a new approach to *a priori* prediction of inorganic compounds which could be used for searching for new electro-optical, ferro-electric, superconducting or semiconducting materials with predefined properties. This approach is based on the use of computer learning strategies.

1.1. Background and Significance

The problem of calculating new multi-element compounds based on knowledge of their constituent element properties seems to be most difficult and still remains unsolved. Prediction based on elemental properties (or simply the listing of desired properties) only is called *a priori* calculation. The difficulties in *a priori* calculation arise from quantum mechanical calculations of multi-electronic systems. An alternative to quantum mechanical calculations is the use of empirical prediction methods in which the existing regularities from a variety of property data are used. Some of these empirical criteria of the predefined properties for compound formation involving the rules of Hume-Rothery [1], Laves [2], Mathias [3], Goldschmidt [4], Villars [5], and Darken-Gurry [6].

The principle objective of finding rules is to identify linear relationships among parameter values of properties associated with constituent elements. Such rules would enable classification of physico-chemical systems into distinct domains. The appeal for such rules is simplicity and consequently the ability to depict information visibly with the help of two-dimensional plots. Often however, classification using two-dimensional plots is deficient, because other properties of the constituent elements come into play, e.g., the thermodynamic phase diagram of a ternary compound. In addition, two-dimensional rules often lose their reliability as new compound, element, and/or property data is introduced which does not easily fit within the rule boundary conditions. The ideal classification scheme must be adaptive, i.e., it must easily accommodate new examples and new property parameters, as well as have a flexible structure and be useful for recognition of any new situation. Such a classification scheme must not be limited by narrow boundaries of two-parameter planes. It is the adaptive, quick, and reliable search of these multidimensional criteria (classification rules) which motivate the following research in computer learning techniques.

[Notes added by A. G. Jackson and S. R. leClair: The process involved consists of the following steps: several classes of compounds are chosen and data on properties of the elements in the compounds is collected. This data constitutes the training set for the pyramidal net algorithm described later. The quantitative data must be quantized, that is, it must be sorted into numerical bins with a given width. Choice of these bins is a rather difficult problem theoretically, and discussion of this problem is not included in this report. Once quantized, the pyramidal net is created producing classification of compounds. A compound not included in the training set can be tested for membership in a class by considering its properties and using the pyramidal net to identify any class it may belong to., including the null class, that is, it does not belong to any class considered or found.

In the research reported in this report the thrust was to predict, using the method described above, the crystal structure type that AB_2Se4 or ABX_2 type compounds belong to for a specific set of possible structure types. The starting information consisted of element data and some information on phase formation. This is the property data referred to above.]

1.2. Preliminary Studies

Our first experiments involving an 'adaptive, multidimensional' computer learning method to search for rules in the formation of binary phases [7] have been very successful. The advantage of using these computer learning methods for multidimensional criteria search is the speed and accuracy resulting from the use of a computer to automate the task of large database analyses and the ability of the computer learning method to quickly classify and re-classify a large, growing set of parameters. This computer learning method has enabled the successful search for the following rules [8-13]: (1) prediction of formation (or non-formation) of compounds for ternary systems; (2) prediction of the possibility of forming ternary and more complicated compounds of desired composition; (3) prediction of phases with definite crystal structures; (4) estimation of phase quantitative properties (critical temperature of transition to a superconducting state, homogeneity region, etc.).

The computer learning method we employ is based upon a cybernetic approach referred to as 'pyramidal-nets' wherein we have predicted the formation of thousands of new compounds in ternary, quaternary and more complicated systems. These compounds were searched to identify new semiconductors, superconductors, ferro-electrics, magnets, and other materials required for new technology [8-13].

> **The comparison of these predictions with the experimental data established [8] an average reliability of the predicted ternary phases exceeding 80% - a higher *a priori* prediction accuracy than by any theoretical method known.**

1.3. Research Design and Methods

In principle there are three ways to predict new electro-optical, ferro-electric, superconducting, and semiconducting inorganic compounds based upon knowledge of their constituent element properties to forecast the intrinsic compound properties:

- **quantum-mechanical calculations;**
- **two-dimensional criteria (classification rules) found by different semi-empirical approaches;**
- **computer learning methods (cybernetic prediction).**

1.4. Methods of Prediction

As a precursor to the cybernetic approach [14] referenced above, multidimensional cybernetic prediction of inorganic compounds was

originally applied by Mendeleev to establish that the periodic change in the properties of chemical systems depends on the properties and nature of the elements which form these systems (compounds, solutions and so on).

Our cybernetic approach has enabled us to reduce the problem of 'new-compound' prediction to the analysis of a multidimensional array of property values and the column vector of the desired property. Each row corresponds to some already known physical-chemical system, i.e., a compound, whose class membership is *a priori* decided by the researcher. The process of analyzing this infomation is aimed at finding regularities or boundaries associated with those compounds within the class. These boundaries are used subsequently to establish whether a new, yet to be evaluated, compound is indeed a member of the class of interest. By substituting the property values of this new compound in the regularity (class boundaries) thus found, it becomes possible to predict the class membership of the new compound. The implementation of this stage (called the "prediction") requires only the knowledge of the values of the component properties.

After testing many methods intended for computer learning applications, we selected an algorithm referred to as Gladun's Algorithm in which all classifying regularities could be presented in the form of a Boolean expression or an equivalent semantic network [14]. We have used this approach on databases of phase properties of ternary inorganic compounds and on the properties of the crystals of acousto-optical, electro-optical, and nonlinear-optical materials to predict new inorganic phases with predefined composition and crystal type which are similar to known electro-optical, ferro-electric, superconducting, magnet, or semiconducting compounds in this research.

[Note (added by Drs LeClair & Jackson):

The Gladun Algorithm is unique as a classification method when compared to various clustering methods including neural networks because it establishes both those attributes which contribute towards defining a class as well as those attributes which, by their exclusion, further define a class.]

2. APPLICATION OF COMPUTER LEARNING METHODS

2.1. Definitions

Physical-chemical system - is a system (e.g., compound, or solid solution) which is formed from chemical elements.

Object - is a physical-chemical system which is described as a set of property (feature) values of the constituent elements.

Feature - is a property of the constituent element of the physical-chemical system.

Learning set - is a multidimensional array of feature values and a column vector of the desired property. Each row corresponds to some physical-chemical system already known, whose class is indicated by row position of the column vector.

Set for prediction - is a multidimensional array of feature values. Each row corresponds to some unknown physical-chemical system, whose class is necessary to predict.

Qualitative property - is an object or element property which can be described as a qualitative concept (e.g., multi-element system with compound formation or non-formation, crystal structure type, possibility of forming compounds of desired composition, and so on).

Quantitative property - is an object or element property which has a numeric value from some continuum (quasi-continuum) set of numbers, (e.g., melting point, birefringence, index of refraction, and so on).

Note: There are two preparatory steps in using computer learning methods:

1) selection of a learning set of compounds which *a priori* have been determined to be within the class of interest and those to be outside of the class of interest;

2) selection of the relevant properties (features) of the constituent elements of those compounds upon which the class boundary will be established.

A problem of selection of the threshold values for the classification arises during the attempt of estimation of unknown quantitative properties (e.g., melting point of compounds). This last problem is similar to the problem of quantization (discretization) of continuous quantitative constituent component properties arising with the use of logical algorithms of computer learning, including Gladun's Algorithm [14].

2.2. Selection of Examples for Computer Learning

The computer learning is carried out on examples of known physical-chemical systems with an *a priori* determination of their belonging to a certain class. If the number of examples in the learning set is not enough and/or examples are not representative of the class of interest, then the resulting classification by regularity describes only that small region of the multidimensional space in which these objects reside. In this case, use of the classification rules for prediction will be unsuccessful. The number and representativeness of the learning set increases if the prediction (estimation) of some unknown quantitative property is desired, e.g., values of birefringence for a chalcopyrite require hundreds of examples in order to obtain acceptable results. Learning set examples which are classified incorrectly introduce large error into the prediction reliability. More specifically, all examples of the incorrectly classified example will be recognized erroneously. Thus, expert assessment of the examples for the learning set is most important.

2.3. Selection of Properties (Features)

The number of element properties (i.e., elements and/or simple compounds) required for compound classification has been studied extensively and is considered to be less than 100. Our research suggests that more important than the number of properties is the selection of properties (herein referred to as features). The selection of those properties which are most representative of the class of interest is the most important consideration for materials scientist.

Gladun's Algorithm of computer learning [14] allows us to identify those properties which have no importance for the classification process, i.e., those properties which do not appear in a rule are not relevant. Thus, it is desirable that the concept formation aspect of Gladun's Algorithm be exercised using a reasonable set of properties. Upon exercise of concept formation those properties which are not relevant can be eliminated from further evaluation. It is necessary to restrict the initial set of properties to a reasonable number on the basis of theoretical physical and chemical grounds by means of expert assessment. An important feature of Gladun's Algorithm [14] which is beneficial for predicting inorganic compound properties is the ability to exercise the algorithm with incomplete property information or ranges where no information exists. It should be noted that if the "gaps" of information regarding a property exceeds 10%, this property should not be selected for classification.

2.4. Selection of Threshold Values for Classification

The problem of computer learning is simplified if the concept or rule sought is formed about a well known class of substances (e.g., the class of physical-chemical systems with elements from a certain composition or definite crystal structure type such as chalcopyrite, perovskite and the like). Clearly all concept formation is "fuzzy", because it is difficult to establish a definitive boundary (threshold value) for the concept of interest.

This fuzziness is characterized by the difficulty of establishing a boundary between similar compounds when processing conditions are unknown, e.g., distinguishing between a pure stoichiometric compound and a non-stoichiometric compound (i.e., with wide homogeneity range in terms of composition) or between spatially varying crystal structures such as an orthorhombically or a tetragonally distorted perovskite and a classic cubic perovskite. Variations in processing conditions, specimen preparation and/or property measurement lead to uncertainty in property data which is unresolved even by qualified experts. In addition, the vagueness of any concept used by a researcher is a source of further inaccuracy of prediction based on computer learning using the learning set.

The problem becomes even more complicated if it is necessary to predict some quantitative property (e.g., the melting point or birefringence of a compound). The hypothesis of class compactness, based on methods of computer learning presupposes that the different classes locate compactly in the multidimensional feature space and there are not intersections between these classes. But we found such a set of properties whose space contradicts this hypothesis. The application of cluster analysis to the example learning set in combination with the grouping of features according to statistical correlation allows us to decrease the intersections of classes, but only slightly, owing to the selection of the natural (for certain learning set) threshold values of predicted quantitative property. Note these natural threshold value are less a consequence of the nature of phases and more the set of examples for the computer learning method. These observations are based upon the learning set examples which have been obtained and investigated at present.

Therefore, as a consequence of the above interaction problem, the attempt to predict certain threshold values which are important for technological

applications, e.g., boiling point temperatures of helium and nitrogen for superconducting compounds, is justified only from a practical standpoint. The error of this prediction will be high, but it will be possible to predict (with high reliability) those properties which are widely spaced in the feature space. *A priori* identification of these properties by a researcher seems to be a great problem. One possibility to solve this problem is to visualize a two-dimensional projection of points, which corresponds to the properties of the learning set, in combination with cluster analysis of properties and grouping features according to statistical correlation. The algorithms for this system involve cluster analysis based on the method of potential functions [15,16] and the extreme grouping of parameters [16]. Both have been applied manually, but implementation for automated use will require more than two manyears of effort.

As stated above, prediction accuracy of quantitative properties depends strongly on the volume and representativeness of the learning set. Our experience shows that the number of learning examples must equal 100s or even 1000s in order to have acceptable estimation of quantitative property.

2.5. Quantization (Discretization) of Continuous Constituent Element Properties

The problem of quantization is a peculiarity of the logical algorithms of the computer learning method. This problem is closely related to the last-mentioned problem of the selection of the threshold values for the computer classification. Quantization is easy to solve if the classification has a qualitative nature (in case of the prediction of qualitative properties). For example, the types of the incomplete electronic shells have four gradation: s-, p-, d-, and f-shell. In the simplest cases, if quantitative properties are integer numbers in the narrow range, it makes sense to assign its gradation to each property value. For example, the number of electrons of the s-shell of the isolated atoms has three gradations: 0, 1 and 2; the formal valency of the element in ionic compounds has eight gradations: 1, 2, 3, 4, 5, 6, 7, and 8.

The problem with the selection of the number of gradations is that they are purely empirical and somewhat arbitrary. It is important to consider that the increase in the number of gradations leads to the decrease in our ability to generalize about the properties of a concept and therein will necessitate an increase of the number of examples in the learning set. At the same time it is obvious that too small a number of gradations leads to the intersection of classes.

It would be ideal if the boundaries between the different feature gradations separate one class of the learning set from another. This idea of solution of the inverse task is a basis of the algorithm of feature quantization which was developed in [17]. At a later time it makes sense to supply the program system of concept formation CONFOR [14] with the programs of the feature preprocessing based on this algorithm [17].

2.6. Ways of Improving the Reliability of Predicting

2.6.1. Utilization of Databases for the Selection of the "Learning Step" Examples

The developed database [18-21] containing ternary compound properties is used for the search information for the computer learning. Our database [20-

23] containing information about the compounds which possess acousto-optical, electro-optical and non-linear optical properties will be used for the search information for the estimation of the properties of substances of this kind. The data about quaternary compounds will be extracted from our card file containing information about the properties of compounds which contain four chemical elements.

2.6.2. Expert Assessment of Data

This is the most difficult problem for the expert who teaches the computer.

2.6.3. Comparison of Predictions Which Have Been Obtained Using Various Property (Feature) Sets

All the properties of chemical elements and compounds are correlated to one another, because they all depend on atomic numbers of elements or combinations of elements (for compounds). In this connection the predictions which have been obtained using different feature sets must be consistent. Lack of consistency is caused by poor quantization of property values and, consequently, by the "fuzzy" boundaries of the concepts which have been formed from the learning set examples. Further, inaccuracy of measurement of the element properties contributes to this fuzziness. However, in individual cases, the lack of consistency may indicate that the learning set examples exhibit a limited set of classes (e.g., the compound has few polymorphous crystal modifications within narrow limits of temperature and pressure).

If the results of prediction, using the different feature sets, contradict one another in the process of the comparison, then the predictions will be rejected in the resulting table, i.e., if the result of prediction using the first feature set is positive, but the result using the second feature set is negative, then the resulting prediction is rejected, and the empty square corresponds to an inconsistency in the resulting table of predictions. When the result of a prediction using the second feature set is vague (designated by an "X" in the table) then it is assumed that the prediction using the first feature set is a true one, i.e. the positive prediction is included in the resulting table.

3. SELECTION OF INORGANIC COMPOUNDS FOR PREDICTION OF NEW ELECTRO-OPTICAL, FERRO-ELECTRIC, SUPERCONDUCTING AND SEMICONDUCTING MATERIALS

3.1. Previous Work Results
3.2. [Empty]
3.3. [Empty]

[Added Note by Drs Jackson and LeClair:

These section numbers were included to retain the original numbering scheme. As opposed to paragraphs of test, these sections reference results from previous work, wherein a number of compounds have been identified as promising candidate materials for specific applications are listed in Tables 3.1, 3.2, and 3.3.]

Table 3.1. Promising Phases for Searching for New Ferro-Electric and Electro-Optical Materials

Composition	Crystal Type	Space Group	Examples	Applications.	Ref.#
ABO_3	Distorted ilmenite	acentric groups	$LiNbO_3$ $LiTaO_3$	E-O Matl's	24
ABO_3	Distorted perovskite	acentric groups	$PbTiO_3$ $BaTiO_3$ $PbZrO_3$ $SrTiO_3$	E-O Matl's	24
AB_2Chal_6	Elpasolith	Fm3m	K_2LiGaF_6	Laser matrix	24
AB_2Chal_4	Th_3P_4	I4(-)3d		E-O Matl's	24
ABX	Chalcopyrite	I4(-)2d	ZnGeP	E-O Matl's	24
AB_2X_4			$CdGa_2S_4$		
A_2BF_6		acentric groups	Ba_2ZnF_6 Sr_2CuF_6	E-O Matl's	24
ABX	PbFCl	P4/nmm	PbFCl	Polarization optics	24
A_3BCl_5		acentric groups	Tl_3PbCl_5	IR-electro-optics	4
ABF_5		acentric groups	$SrAlF_5$	Laser matrix	24
$A_2BC_2O_7$	Melilite	P4(-)2 m	$Ba_2ZnGe_2O_7$ $Ba_2ZnGe_2O_7$	Laser matrix	24

Table 3.2. Promising Phases for Searching for New Semiconductors and Magnet Semiconductors

Composition	Crystal Type	Space Group	Examples	Applications	Ref#
AB_2Se_4	Spinel	Fd3m	$CdCr_2Se_4$	Data storage and processing devices, magneto-optics, non-linear capacitors, microwave, integrated circuits, and so on	25

Table 3.3. Phases Which Hold the Promise for Searching for New Superconductors

Composition	Crystal Type	Space Group	Examples	Applications	Ref#
$R_x R'_{1-x}CuO_4$	CuO	T'	$Nd_xCe_{2-x}CuO_4$	Electron-doped Hi temperature Superconductor	26,27
AB_2Chal_4	Spinel	Fd3m $CuRh_2S_4$ CuV_2S_4	$CuRh_2Se_4$	Superconductors	32

3.4. Predicting New Compounds of Composition AB_2Se_4 with Crystal Structure Types of Th_3P_4 Chalcopyrite, Spinel, and etc.

Phases with crystal type Th_3P_4 (space group I4(-)3d) [29,31] are of interest for compounds which hold promise for new semiconducting and electro-optical materials [24,25]. We attempted to predict the new chalcopyrite (space group I4(-)2d) [28,29] of composition AB_2Se_4 (the Examples of promised compound $CdGa_2S_4$ with interesting electro-optical properties) [24].

In searching for new semiconductors, superconductors, and magnetic semiconductors, we attempted to predict new selenides of composition AB_2Se_4 and spinel crystal type (space group Fd3m) [25,29,31-34]. These compounds are of interest for development of data storage and processing devices, magneto-optics, non-linear capacitors, microwave integrated circuits, and so on [25].

3.4.1. Data for Computer Learning.

The data for computer learning was extracted from the DB on ternary inorganic compound properties [18-21]. We had predicted the new selenides of this composition and with structure types spinel [8, 36], Th_3P_4, $CaFe_2O_4$, and $NiCr_2Se_4$ previously [8]. In this investigation all information for the computer learning was assessed by expert on the inorganic compounds of selenium Dr. T. I. Koneshova (Kurnakov Institute of General and Inorganic Chemistry of RAN). The table 3.4.1 contains a resulting learning set.

At first we predicted the possibility of forming compounds of composition AB_2Se_4 (divided into two classes - dichotomy). Next, we predicted the crystal types (chalcopyrite [28,29], spinel [25,29,31-34], Th_3P_4 [24,25,31], $PbGa_2Se_4$ space group Cccm) [30], Yb_3S_4 (space group Cmc2), Yb_3Se_4 (rhombohedral structure), $CaFe_2O_4$ (space group Pnam), $NiCr_2Se_4$ (space group C2/m), and olivine (space group Pbnm)) at standard conditions (at room temperature and normal pressure) for predicted on the first stage compounds (multiclass predicting).

Table 3.4.1 Learning set for Predicting Crystal Types with Composition AB_2Se_4

Composition	Crystal type
$GeHg_2Se_4$	chalcopyrite
$ZnAl_2Se_4$	chalcopyrite
$CdAl_2Se_4$	chalcopyrite
$ZnGa_2Se_4$	chalcopyrite
$ZnIn_2Se_4$	chalcopyrite
$CdGa_2Se_4$	chalcopyrite
$HgGa_2Se_4$	chalcopyrite
$CdIn_2Se_4$	chalcopyrite
$HgIn_2Se_4$	chalcopyrite
$SnMg_2Se_4$	olivine
$SiCa_2Se_4$	olivine
$SiMn_2Se_4$	olivine
VTi_2Se_4	$NiCr_2Se_4$
$CoSi_2Se_4$	$NiCr_2Se_4$
$NiSi_2Se_4$	$NiCr_2Se_4$
$TiCr_2Se_4$	$NiCr_2Se_4$
$CrTi_2Se_4$	$NiCr_2Se_4$
$MnTi_2Se_4$	$NiCr_2Se_4$
$TiFe_2Se_4$	$NiCr_2Se_4$
$FeTi_2Se_4$	$NiCr_2Se_4$
$CoTi_2Se_4$	$NiCr_2Se_4$
$NiTi_2Se_4$	$NiCr_2Se_4$
MnV_2Se_4	$NiCr_2Se_4$
VFe_2Se_4	$NiCr_2Se_4$
FeV_2Se_4	$NiCr_2Se_4$
NiV_2Se_4	$NiCr_2Se_4$
$NiCr_2Se_4$	$NiCr_2Se_4$
$TiTi_2Se_4$	$NiCr_2Se_4$
VV_2Se_4	$NiCr_2Se_4$
$CrCr_2Se_4$	$NiCr_2Se_4$
$FeFe_2Se_4$	$NiCr_2Se_4$
$CrRh_2Se_4$	$NiCr_2Se_4$
$CoRh_2Se_4$	$NiCr_2Se_4$
$NiRh_2Se_4$	$NiCr_2Se_4$
$FeGa_2Se_4$	spinel
$MnSc_2Se_4$	spinel
$CuCr_2Se_4$	spinel
$ZnCr_2Se_4$	spinel
$CdCr_2Se_4$	spinel
$HgCr_2Se_4$	spinel

Composition	Crystal type
$CuMn_2Se_4$	spinel
$ZnMn_2Se_4$	spinel
$CuRh_2Se_4$	spinel
CdY_2Se_4	spinel
$CdDy_2Se_4$	spinel
$CdHo_2Se_4$	spinel
$CdEr_2Se_4$	spinel
$CdTm_2Se_4$	spinel
$CdYb_2Se_4$	spinel
$CdLu_2Se_4$	spinel
$SrAl_2Se_4$	$PbGa_2Se_4$
$EuAl_2Se_4$	$PbGa_2Se_4$
$YbAl_2Se_4$	$PbGa_2Se_4$
$PbAl_2Se_4$	$PbGa_2Se_4$
$CaGa_2Se_4$	$PbGa_2Se_4$
$SrGa_2Se_4$	$PbGa_2Se_4$
$BaGa_2Se_4$	$PbGa_2Se_4$
$EuGa_2Se_4$	$PbGa_2Se_4$
$YbGa_2Se_4$	$PbGa_2Se_4$
$PbGa_2Se_4$	$PbGa_2Se_4$
$SmIn_2Se_4$	$PbGa_2Se_4$
$EuIn_2Se_4$	$PbGa_2Se_4$
$YbIn_2Se_4$	$PbGa_2Se_4$
$CrLa_2Se_4$	Th_3P_4
$CrCe_2Se_4$	Th_3P_4
$CrPr_2Se_4$	Th_3P_4
$CrNd_2Se_4$	Th_3P_4
$CrSm_2Se_4$	Th_3P_4
$CrEu_2Se_4$	Th_3P_4
$PbLa_2Se_4$	Th_3P_4
$PbCe_2Se_4$	Th_3P_4
$PbPr_2Se_4$	Th_3P_4
$PbNd_2Se_4$	Th_3P_4
$PbSm_2Se_4$	Th_3P_4
$SmNd_2Se_4$	Th_3P_4
$SmSm_2Se_4$	Th_3P_4
$CdLa_2Se_4$	Th_3P_4
$CdPr_2Se_4$	Th_3P_4
$CdGd_2Se_4$	Th_3P_4
$EuLa_2Se_4$	Th_3P_4

Composition	Crystal type
$EuCe_2Se_4$	Th_3P_4
$EuPr_2Se_4$	Th_3P_4
$EuNd_2Se_4$	Th_3P_4
$EuSm_2Se_4$	Th_3P_4
$EuGd_2Se_4$	Th_3P_4
$EuTb_2Se_4$	Th_3P_4
$CeCe_2Se_4$	Th_3P_4
$PrPr_2Se_4$	Th_3P_4
$NdNd_2Se_4$	Th_3P_4
ULa_2Se_4	Th_3P_4
UCe_2Se_4	Th_3P_4
UPr_2Se_4	Th_3P_4
UNd_2Se_4	Th_3P_4
USm_2Se_4	Th_3P_4
UGd_2Se_4	Th_3P_4
UU_2Se_4	Th_3P_4
$NpNp_2Se_4$	Th_3P_4
$PuPu_2Se_4$	Th_3P_4
$AmAm_2Se_4$	Th_3P_4
CaY_2Se_4	Yb_3S_4
$CaHo_2Se_4$	Yb_3S_4
$YbHo_2Se_4$	Yb_3S_4
$YbEr_2Se_4$	Yb_3S_4
$YbTm_2Se_4$	Yb_3S_4
$CaDy_2Se_4$	Yb_3Se_4
$CaEr_2Se_4$	Yb_3Se_4
$CaYb_2Se_4$	Yb_3Se_4
$CaLu_2Se_4$	Yb_3Se_4
$YbYb_2Se_4$	Yb_3Se_4
$EuSc_2Se_4$	$CaFe_2O_4$
SrY_2Se_4	$CaFe_2O_4$
$SrTb_2Se_4$	$CaFe_2O_4$
$SrDy_2Se_4$	$CaFe_2O_4$
$SrHo_2Se_4$	$CaFe_2O_4$
$SrEr_2Se_4$	$CaFe_2O_4$
$SrTm_2Se_4$	$CaFe_2O_4$
$SrYb_2Se_4$	$CaFe_2O_4$
$SrLu_2Se_4$	$CaFe_2O_4$
BaY_2Se_4	$CaFe_2O_4$
$BaSm_2Se_4$	$CaFe_2O_4$

Composition	Crystal type
$BaGd_2Se_4$	$CaFe_2O_4$
$BaDy_2Se_4$	$CaFe_2O_4$
$BaYb_2Se_4$	$CaFe_2O_4$
$BaLu_2Se_4$	$CaFe_2O_4$
$EuHo_2Se_4$	$CaFe_2O_4$
$EuEr_2Se_4$	$CaFe_2O_4$
$EuTm_2Se_4$	$CaFe_2O_4$
$EuYb_2Se_4$	$CaFe_2O_4$
$EuLu_2Se_4$	$CaFe_2O_4$
$PbEr_2Se_4$	$CaFe_2O_4$
$PbTm_2Se_4$	$CaFe_2O_4$
$PbYb_2Se_4$	$CaFe_2O_4$
$PbLu_2Se_4$	$CaFe_2O_4$

Table 3.4.1. (Continued) with the addition of Space Group and Number of Formula Units (Z)

Composition	Crystal type	Space group	Z
$SiBa_2Se_4$	$GeSr_2S_4$	P2(1)/m	2
$FeSi_2Se_4$	CdI2		
$GeZn_2Se_4$	ZnS		
$GeCd_2Se_4$	$GeCd_2S_4$	rhombohedral	9
$GeEu_2Se_4$	$GeSr_2S_4$	P2(1)/m	2
$GeYb_2Se_4$	$GeSr_2S_4$	P2(1)/m	2
$SnHg_2Se_4$	I4(-)		
$MgAl_2Se_4$	R3m		
$MgIn_2Se_4$	R3m		
$BaAl_2Se_4$	P4/nnc		4
$CaIn_2Se_4$	P2(1)2(1)2(1)		4
SrV_2Se_4	hexagonal		
EuV_2Se_4	hexagonal		9
$SrCr_2Se_4$	hexagonal		
$BaCr_2Se_4$	hexagonal		
$EuCr_2Se_4$	$PbCr_2S_4$	P6	9
$CrTb_2Se_4$	rhombic		12
$CrDy_2Se_4$	rhombic		12
$CrLu_2Se_4$	rhombic		12
$PbCr_2Se_4$	hexagonal		
$MnGa_2Se_4$	ZnS		
$MnAs_2Se_4$	tetragonal		2
$MnBi_2Se_4$	tetragonal		
$CdTl_2Se_4$	hexagonal		
$SnSb_2Se_4$	Pnnm		12
$SnNd_2Se_4$	Fdd2		16
$BaSb_2Se_4$	P2(1)/n		8
$EuSb_2Se_4$	$PbBi_2S_4$	P2(1)2(1)2(1)	
$BaBi_2Se_4$	P6(3)/m		12
$CuGa_2Se_4$	ZnS		

Table 3.4.1.a. Pseudo-Binary Systems with Se anions in which AB_2Se_4 is not formed.

$ZnSe-SnSe_2$	without compound AB_2Se_4	$YbSe-Gd_2Se_3$	without compound AB_2Se_4
$GaSe-GeSe_2$	without compound AB_2Se_4	$YbSe-Tb_2Se_3$	without compound AB_2Se_4
$InSe-GeSe_2$	without compound AB_2Se_4	$YbSe-Dy_2Se_3$	without compound AB_2Se_4
$SnSe-GeSe_2$	without compound AB_2Se_4	$SnSe-Ga_2Se_3$	without compound AB_2Se_4
$CdSe-SnSe_2$	without compound AB_2Se_4	$CdSe-Sn_2Se_3$	without compound AB_2Se_4
$TlSe-SnSe_2$	without compound AB_2Se_4	$TlSe-Ga_2Se_3$	without compound AB_2Se_4
$SnSe_2-AuSe$	without compound AB_2Se_4	$GaSe-Tl_2Se_3$	without compound AB_2Se_4
$SnSe_2-InSe$	without compound AB_2Se_4	$GeSe-Sb_2Se_3$	without compound AB_2Se_4
$USe-Sc_2Se_3$	without compound AB_2Se_4	$CdSe-As_2Se_3$	without compound AB_2Se_4
$USe-Ho_2Se_3$	without compound AB_2Se_4	$NdSe-As_2Se_3$	without compound AB_2Se_4
$USe-Er_2Se_3$	without compound AB_2Se_4	$HgSe-As_2Se_3$	without compound AB_2Se_4
$USe-Tm_2Se_3$	without compound AB_2Se_4	$SnSe-In_2Se_3$	without compound AB_2Se_4
$USe-Lu_2Se_3$	without compound AB_2Se_4	$SnSe-Au_2Se_3$	without compound AB_2Se_4
$USe-Y_2Se_3$	without compound AB_2Se_4	$SnSe-Bi_2Se_3$	without compound AB_2Se_4
$GaSe-As_2Se_3$	without compound AB_2Se_4	$HgSe-Sb_2Se_3$	without compound AB_2Se_4
$CuSe-Nd_2Se_3$	without compound AB_2Se_4	$HgSe-Bi_2Se_3$	without compound AB_2Se_4
$CuSe-Gd_2Se_3$	without compound AB_2Se_4	$CrSe-In_2Se_3$	without compound AB_2Se_4
$SmSe-As_2Se_3$	without compound AB_2Se_4	$CoSe-In_2Se_3$	without compound AB_2Se_4
$YbSe-Ce_2Se_3$	without compound AB_2Se_4	$CuSe-In_2Se_3$	without compound AB_2Se_4
$YbSe-Pr_2Se_3$	without compound AB_2Se_4	$ZnSe-Bi_2Se_3$	without compound AB_2Se_4
$YbSe-Nd_2Se_3$	without compound AB_2Se_4	$GeSe-Ga_2Se_3$	without compound AB_2Se_4
$YbSe-Eu_2Se_3$	without compound AB_2Se_4	$GeSe-In_2Se_3$	without compound AB_2Se_4

3.4.2. Selection of of Features.

On the basis of physical-chemical grounds three sets of constituent component features were selected for the description of selenide systems and compounds.

3.4.2.1. Feature Set I.

Set I includes information about the number of electrons in energy shells of separate atoms, the covalent radii, and the formal valence of elements A or B in the compound of composition AB_2Se_4. The grouping of energy shell information (hereafter referred to as gradation) corresponds to the number of electrons for each shell and their respective valence value. The quasi-continuous property - the covalent radius - was divided (quantized) on the basis of the uniform distribution of the values of the intervals. Table 3.4.2 contains the gradations for Feature Set I.

3.4.2.2. Feature Set II.

Set II includes the following information: the first three ionization potentials, the electronegatives, the types of incomplete electronic shells, the number of electrons in the incomplete electronic shell, the covalent or metallic radii, the ratio of the atomic number to the average atomic mass for atoms of elements A and B, the standard enthalpies of formation of corresponding simple selenides, the number of the group in Periodic Table and the formal valences exhibited in an AB_2Se_4 compound. The quantitative properties (ionization potentials, the electronegativities, the covalent or metallic radii, the standard enthalpies of formation) were quantized on the basis of the uniform distribution of the values of the intervals. Table 3.4.3 contains the gradations for Feature Set II.

3.4.2.3. Feature Set III.

Feature Set III includes the following information: the covalent or metallic radii for the elements A and B, the standard enthalpies of formation of corresponding simple selenides, and the standard entropies of simple selenides. These quantitative properties were quantized on the basis of uniform distribution of the values of the intervals. Table 3.4.4 contains the gradations for the Feature Set III.

Table 3.4.2 Gradations for the Feature Set I

Feature	Gradation	Feature	Gradation
1s-shell		5d-shell	
s1	S11	d0	D50
s2	S12	d1	D51
2s-shell		d2	D52
s0	S20	d3	D53
s1	S21	d4	D54
s2	S22	d5	D55
2p-shell		d6	D56
p0	P20	d7	D57
p1	P21	d9	D59
p2	P22	d10	D510
p3	P23	5f-shell	
p4	P24	f0	F50
p5	P25	f2	F52
p6	P26	f3	F53
3s-shell		f4	F54
s0	S30	f5	F55
s1	S31	f6	F56
s2	S32	f7	F57
3p-shell		f9	F58
p0	P30	f10	F510
p1	P31	f11	F511
p2	P32	f12	F512
p3	P33	f13	F513
p4	P34	f14	F514
p5	P35	6s-shell	
p6	P36	s0	S60
3d-shell		s1	S61
d0	D30	s2	S62
d1	D31	6p-shell	
d2	D32	p0	P60
d3	D33	p1	P61
d4	D34	p2	P62
d5	D35	p3	P63
d6	D36	p4	P64
d7	D37	p5	P65
d8	D38	p6	P66
d10	D310	6d-shell	
4s-shell		d0	D60
s0	S40	d1	D61
s1	S41	d2	D62
s2	S42	7s-shell	
4p-shell		s0	S70

Feature	Gradation	Feature	Gradation
p0	P40	s1	S71
p1	P41	s2	S72
p2	P42	Valency	
p3	P43	+1	B1
p4	P44	+2	B2
p5	P45	+3	B3
p6	P46	+4	B4
4d-shell		+5	B5
d0	D40	+6	B6
d1	D41	+7	B7
d2	D42	+8	B8
d3	D43	Covalent or	
d4	D44	metallic	
d5	D45	radius,A	
d6	D46	[0.028-1.04]	R1
d7	D47	[1.04-1.3]	R2
d8	D48	[1.3-1.36]	R3
d10	D410	[1.36-1.43]	R4
4f-shell		[1.43-1.58]	R5
f0	F40	[1.58-1.62]	R6
f2	F42	[1.62-1.75]	R7
f3	F43	[1.75-1.82]	R8
f4	F44	[1.82-1.88]	R9
f5	F45	[1.88-2.80]	R10
f6	F46		
f7	F47		
f9	F48		
f10	F410		
f11	F411		
f12	F412		
f13	F413		
f14	F414		
5s-shell			
s0	S50		
s1	S51		
s2	S52		
5p-shell			
p0	P50		
p1	P51		
p2	P52		
p3	P53		
p4	P54		
p5	P55		
p6	P56		

Table 3.4.3 Gradations for Feature Set II

Feature	Gradation	Feature	Gradation
Type of incomplete electronic shell		Ratio of the atomic number to the average atomic mass, 1/c.u.	
s	S	0.99	NM1
p	P	0.50	NM2
d	D	0.49	NM3
f	F	0.48	NM4
Electronegative		0.47	NM5
[0.7-1]	Ne1	0.46	NM6
[1-1.2]	Ne2	0.45	NM7
[1.2-1.3]	Ne3	0.44	NM8
[1.3-1.6]	Ne4	0.43	NM9
[1.6-1.8]	Ne5	0.42	NM10
[1.8-1.9]	Ne6	0.41	NM11
[1.9-2.1]	Ne7	0.40	NM12
[2.1-2.2]	Ne8	0.39	NM13
[2.2-4]	Ne9		
First ionization potential, eV		Number of electrons on incomplete electronic shell	
[3.893-5.39]	I11		
[5.39-5.90]	I12		
[5.90-6.31]	I13		
[6.31-6.74]	I14	0	E0
[6.74-6.95]	I15	1	E1
[6.95-7.432]	I16	2	E2
[7.432-7.87]	I17	3	E3
[7.87-8.64]	I18	4	E4
[8.64-9.30]	I19	5	E5
[9.30-10.55]	I110	6	E6
[10.55-25]	I111	7	E7
		8	E8
Second ionization potential, eV		9	E9
		10	E10
[0-11.5]	I21	11	E11
[11.5-12.4]	I22	12	E12
[12.4-14.2]	I23	13	E13
[14.2-15.92]	I24		
[15.92-16.904]	I25	Number of group	
[16.904-18.7]	I26	1	N1
[18.7-19.65]	I27	2	N2
[19.65-21.5]	I28	3	N3
[21.5-27.56]	I29	4	N4
[27.56-75.62]	I210	5	N5
		6	N6
Third ionization potential, eV		7	N7
		8	N8
[0-21]	I31		
[21-24]	I32	Standard enthalpy of formation for corresponding simple selenide, kcal/mol	
[24-25.61]	I33		
[25.61-29]	I34		
[29-30.64]	I35		
[30.64-32.8]	I36		
[32.8-34.21]	I37		
[34.21-37]	I38	[-66 - -12.2]	H1
[37-47.426]	I39	[-12.2 - -8]	H2
[47.426-154]	I310	[-8 - 0]	H3
		[0 - 14]	H4
Covalent or metallic radius, A		[14 - 18]	H5
		[18 - 24.5]	H6
[0.28-1.04]	R1	[24.5 - 36.64]	H7
[1.04-1.21]	R2	[36.64 - 50.8]	H8
[1.21-1.25]	R3	[50.8 - 82]	H9
[1.25-1.26]	R4	[82 - 223]	H10
[1.26-1.27]	R5		
[1.27-1.30]	R6	Formal valency	
[1.30-1.34]	R7	1	Se21
[1.34-1.37]	R8	2	Se11
[1.37-1.38]	R9	3	Se23
[1.38-1.40]	R10	4	Se12
[1.40-1.44]	R11	5	Se13
[1.44-1.54]	R12		
[1.54-1.75]	R13		
[1.75-1.82]	R14		
[1.82-1.83]	R15		
[1.83-1.87]	R16		
[1.87-2.8]	R17		

Table 3.4.4 Gradations for the Feature Set III

Feature	Gradation	Feature	Gradation
Type of incomplete electronic shell		Standard enthalpy of formation for corresponding simple selenide, kcal/mol	
s	S		
p	P		
d	D		
f	F		
		[-66 - -12.2]	H1
Electronegative		[-12.2 - -8]	H2
[0.7-1]	Ne1	[-8 - 0]	H3
[1-1.2]	Ne2	[0 - 14]	H4
[1.2-1.3]	Ne3	[14 - 18]	H5
[1.3-1.6]	Ne4	[18 - 24.5]	H6
[1.6-1.8]	Ne5	[24.5 - 36.64]	H7
[1.8-1.9]	Ne6	[36.64 - 50.8]	H8
[1.9-2.1]	Ne7	[50.8 - 82]	H9
[2.1-2.2]	Ne8	[82 - 223]	H10
[2.2-4]	Ne9		
		Standard entropy for corresponding simple selenide, cal/mol*K	
Covalent or metallic radius, A			
[0.28-1.21]	R1		
[1.21-1.26]	R2		
[1.26-1.30]	R3	[1-15.7]	S1
[1.30-1.37]	R4	[15.7-18]	S2
[1.37-1.40]	R5	[18-19.2]	S3
[1.40-1.54]	R6	[19.2-20.74]	S4
[1.54-1.82]	R7	[.0.74-22.5]	S5
[1.82-1.87]	R8	[22.5-24.5]	S6
[1.87-2.8]	R9	[24.5-26.9]	S7
		[26.9-39]	S8
Formal Valency		[39-53.2]	S9
0	B0	[53.2-96]	S10
1	B1		
2	B2		
3	B3		
4	B4		
5	B5		
6	B6		
7	B7		
8	B8		

3.4.3. Prediction of Formation.

In the case of predicting the formation of the compounds with composition AB_2Se_4 the computer learning is carried-out for three learning sets in which the compounds from Table 3.4.1 were described in terms of the sets of the component properties I-III. The system of concept formation CONFOR [14] was used for computer learning and prediction.

Since computer memory capacity for the storage of semantic networks for the learning sets in terms of I and II became more than 65,500 symbols, the corresponding learning sets were divided into two sets: for the compounds of formally two- and four-valence elements and for the compounds of formally two- and three-valence elements.

3.4.4. Prediction of Crystal Structure.

In the case of predicting the crystal type of the compounds with composition AB_2Se_4 computer learning was carried out for three learning sets in which the compounds from Table 3.4.1 were described in terms of the sets of the component features I-III. The system of concept formation, CONFOR, [14] was used for computer learning and predicting.

Again, the problem of computer memory capacity for storage of semantic net for the learning sets in the terms of I and II arises, the learning process was divided into two stages: for the compounds of formally two- and four-valence elements and for the compounds of formally two- and three-valence elements.

The pyramidal networks and the corresponding logical expressions were formed as a result of the computer learning via CONFOR. Appendix 1 contains the logical expressions for various learning sets. Hereafter, the following conventional signs are used: V - a disjunction sign, * - a conjunction sign, and *~, or *-, or -* - a negation sign. The number in square brackets is the number of iterations of a fragment of the logical expression in a learning set.

3.4.5. Descriptions in terms of Learning Set I.

In the case of the descriptions in terms of Learning Set I, some of the objects from Table 3.4.1 were selected for the examination. The results of examination testify (Table 3.4.5) that there is a vagueness of recognition which suggests that the level of the computer training, in the case of the description in terms of the distribution of electrons in the shells of separate atoms, the covalent radii, and the corresponding formal valence, is rather bad (Table 3.4.6).

Table 3.4.5 Set for Examination

Composition	Crystal type	Result of examination
$CdAl_2Se_4$	chalcopyrite	X
$ZnGa_2Se_4$	chalcopyrite	X
$CdCr_2Se_4$	PINELX	X
$CdHo_2Se_4$	PINELX	X
$CdEr_2Se_4$	PINELX	X
$SrGa_2Se_4$	$PbGa_2Se_4$	X
$YbGa_2Se_4$	$PbGa_2Se_4$	X
$CrTi_2Se_4$	$NiCr_2Se_4$	$NiCr_2Se_4$
$CoTi_2Se_4$	$NiCr_2Se_4$	X
$CrPr_2Se_4$	Th_3P_4	X
$PbNd_2Se_4$	Th_3P_4	X
$CdPr_2Se_4$	Th_3P_4	X
$EuCe_2Se_4$	Th_3P_4	X
$EuGd_2Se_4$	Th_3P_4	X
$YbTm_2Se_4$	Yb_3S_4	Yb_3S_4
$CaEr_2Se_4$	Yb_3Se_4	X
$SrDy_2Se_4$	$CaFe_2O_4$	X
$SrYb_2Se_4$	$CaFe_2O_4$	X
$BaGd_2Se_4$	$CaFe_2O_4$	X
$BaYb_2Se_4$	$CaFe_2O_4$	X
$PbTm_2Se_4$	$CaFe_2O_4$	X
$CrDy_2Se_4$	another structure	X
$YbSe\text{-}Pr_2Se_3$	without AB_2Se_4	without AB_2Se_4
$YbSe\text{-}Sm_2Se_3$	without AB_2Se_4	X
$YbSe\text{-}Dy_2Se_3$	without AB_2Se_4	without AB_2Se_4

Table 3.4.6
ESTIMATION OF RESULTS OF EXAMINATION

Class of chalcopyrite
- number of objects 2 ;
- correctly 0 [0 %] ;
- incorrectly 0 [0 %] ;
- indeterminately 2 [100 %] ;

Class of spinel
- number of objects 3 ;
- correctly 0 [0 %] ;
- incorrectly 0 [0 %] ;
- indeterminately 3 [100 %] ;

Class of $PbGa_2Se_4$:
- number of objects 2 ;
- correctly 0 [0 %] ;
- incorrectly 0 [0 %] ;
- indeterminately 2 [100 %] ;

Class of $NiCr_2Se_4$:
- number of objects 2 ;
- correctly 1 [50 %] ;
- incorrectly 0 [0 %] ;
- indeterminately 1 [50 %] ;

Class of Th_3P_4 :
- number of objects 5 ;
- correctly 0 [0 %] ;
- incorrectly 0 [0 %] ;
- indeterminately 5 [100 %] ;

Class of Yb_3S_4 :
- number of objects 1 ;
- correctly 1 [100 %] ;
- incorrectly 0 [0 %] ;
- indeterminately 0 [0 %] ;

Class of Yb_3Se_4 :
- number of objects 1 ;
- correctly 0 [0 %] ;
- incorrectly 0 [0 %] ;
- indeterminately 1 [100 %] ;

Class of $CaFe_2O_4$:
- number of objects 5 ;
- correctly 0 [0 %] ;
- incorrectly 0 [0 %] ;
- indeterminately 5 [100 %] ;

Class of another structure :
- number of objects 1 ;
- correctly 0 [0 %] ;
- incorrectly 0 [0 %] ;
- indeterminately 1 [100 %] ;

Class without compound AB_2Se_4 :
- number of objects 3 ;
- correctly 2 [66.666667 %] ;
- incorrectly 0 [0 %] ;
- indeterminately 1 [33.333333 %] ;

Number of objects 25 ;
correctly 4 [16 %] ;
incorrectly 0 [0 %] ;
indeterminately 21 [84 %].

3.4.6. Predictions of Crystal Structure.

The table of predictions of the crystal structure type for the compounds of composition $A(II)B(III)_2Se_4$ (Table 3.4.7) results from comparison of the results of prediction with use of the descriptions in terms of the Feature Sets I-III (see Section 2.6.3). The following designations are used:

S - spinel;
C - chalcopyrite
P - $PbGa_2Se_4$
Y - Yb_3S_4
E - Yb_3Se_4
F - $CaFe2O_4$
T - Th_3P_4
O - olivine
N - $NiCr_2Se_4$
- - the crystal structure differing from those listed above;
* - the compound of composition AB_2Se_4 does not form.

The physical-chemical systems, which were investigated experimentally, [designated by a symbol + * or **]. The empty square corresponds to the lack of coincidence of the predictions, which have been obtained using different feature sets. According to our results the new compounds of the composition $A(IV)B(II)_2Se_4$ with the crystal structure of the chalcopyrite, spinel, or In_3P_4 at normal pressure and room temperature don't exist. The analysis of Table 3.4.7 shows: it is unlikely that the new compounds of the composition $A(II)B(III)_2Se_4$ with the crystal structure of the chalcopyrite or spinel form at normal pressure for the combinations of elements A and B which are indicated in this Table. At the same time the great number of predictions of new compounds with crystal structure type Th_3P_4, which hold the promise for searching for new electro-optical materials, were obtained.

Table 3.4.7 Table of Predictions of Crystal for Compounds of Composition A(II)B(III)$_2$Se$_4$

B:	Al	Sc	Cr	Ga	Y	In	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Tl
A																						
Mg	-					-	T															
Ca	P*			P*	Y*	- *	T									E *	Y*	E *		E*	E*	
Ti		N	N*																			
V		N	N*																			
Cr		N	N*		* *	T*	T*	T *	T*		T*	T*		- *	- *					- *		
Mn		S*		- *		- *	T															
Fe		N		S *		*																
Co						* *																
Ni			N*																			
Cu			S*	- *		* *				* *				* *						*		
Zn	C*		S*	C*		C*	T															
Sr	P*		- *	P *	F		T								F*	F*	F*	F*	F*	F*	F*	
Y	T*				T*		T	T	T			T								* *	T *	
Cd	C		S*	C*	S*	C*	T*		T*					T *		S*	S*	S*	S*	S*	S*	- *
Ba	- *		- *	P*	F*		T					F*		F*		F*				F*	F*	-
La		T	T					T	T			T			F	F	F	F				F
Ce		T			T		T	T*	T		T	T	T		T	T	T	T	T	*		
Pr		T			T		T	T*	T*		T	T	T		T	T	T	T	T	*		
Nd										T*										*		
Pm		F						T	T										F			
Sm		T	T			P *	T	T	T	T*	T	T*	T		T							T
Eu	P *	F*	- *	P *		P *	T*	T*	T*	T*		T*	F	T*	T*		F*	F*	F*	F*	F*	F
Gd												T	T									
Tb		F					F	T	T			T			F	F	F	F	F	*	F	
Dy		F					F	T	T			T	F		F	F	F	F	F	*	F	
Ho		F					F	T	T			T	F		F	F	F	F	F		F	
Er		F					F	T	T			T	F		F	F	F	F	F		F	
Tm		F						T	T						F	F	F	F	F			
Yb	P *			P *		P *		* *	* *	* *		* *	* *	* *	* *	* *	Y*	Y*	Y*	E*		Y
Lu		T					T					T	F		F	F	F	F			T	
Hg			S*	C*		C*							F					P	P		F	
Pb	P *		-	P			T*	T*	T*	T*		T*	F	F	F			F*	F*	F*	F*	*

3.5. Prediction of the New Compounds of Composition ABX_2

The class of compounds with structure resembling that of chalcopyrite holds the greatest promise for searching for the new electro-optical and semiconducting materials [24,35]. We had attempted to predict new chalcopyrites previously [37].

3.5.1. Prediction of New Chalcopyrites of Composition ABX_2,

Prediction of New Chalcopyrites of Composition ABX_2 where:

A = Li, Na, K, Rb, Cs, Cu, Ag, Au, Zn, Cd, Hg;
B = Al, Ga, In, Tl, Fe, Co, Ni; X = O, S, Se, Te).

3.5.1.1. Data for Computer Learning.

The data for computer learning was extracted from the database on ternary inorganic compound properties [18-21]. In this investigation we attempted to predict new compounds with the composition given above which have the crystal structure resembling the chalcopyrite (space group I4(-)2d) [35], a-$NaFeO_2$ (space group R3m) [29], b-$NaFeO_2$ (space group Pna2), TlSe (space group I4/mcm) [38], or a-$LiFeO_2$ (space group I4/amd) at normal pressure and room temperature. Table 3.5.1 contains a learning set.

Table 3.5.1 Learning set for Prediction of Crystal Types of Compounds with Composition ABX_2

Composition	Crystal type
$LiInTe_2$	chalcopyrite
$CuAlS_2$	chalcopyrite
$CuAlSe_2$	chalcopyrite
$CuAlTe_2$	chalcopyrite
$CuGaS_2$	chalcopyrite
$CuGaSe_2$	chalcopyrite
$CuGaTe_2$	chalcopyrite
$CuInS_2$	chalcopyrite
$CuInSe_2$	chalcopyrite
$CuInTe_2$	chalcopyrite
$CuTlS_2$	chalcopyrite
$CuTlSe_2$	chalcopyrite
$CuTlTe_2$	chalcopyrite
$CuFeS_2$	chalcopyrite
$CuFeSe_2$	chalcopyrite
$CuFeTe_2$	chalcopyrite
$AgAlS_2$	chalcopyrite
$AgAlSe_2$	chalcopyrite
$AgAlTe_2$	chalcopyrite
$AgGaS_2$	chalcopyrite
$AgGaSe_2$	chalcopyrite
$AgGaTe_2$	chalcopyrite
$AgInS_2$	chalcopyrite
$AgInSe_2$	chalcopyrite
$AgInTe_2$	chalcopyrite
$AgTlSe_2$	chalcopyrite
$AgTlTe_2$	chalcopyrite
$AgFeO_2$	chalcopyrite
$AgFeS_2$	chalcopyrite
$AgFeSe_2$	chalcopyrite
$AgFeTe_2$	chalcopyrite
$ZnAlS_2$	chalcopyrite
$ZnAlSe_2$	chalcopyrite
$ZnAlTe_2$	chalcopyrite
$ZnGaTe_2$	chalcopyrite
$ZnTlTe_2$	chalcopyrite
$CdGaTe_2$	chalcopyrite
$HgGaTe_2$	chalcopyrite
$LiAlS_2$	β-$NaFeO_2$
$LiGaO_2$	β-$NaFeO_2$
$LiInSe_2$	β-$NaFeO_2$
$NaAlO_2$	β-$NaFeO_2$
$NaGaO_2$	β-$NaFeO_2$
$LiAlO_2$	α-$NaFeO_2$
$LiNiO_2$	α-$NaFeO_2$
$NaInS_2$	α-$NaFeO_2$
$NaInSe_2$	α-$NaFeO_2$
$NaInO_2$	α-$NaFeO_2$
$NaTlO_2$	α-$NaFeO_2$
$NaFeO_2$	α-$NaFeO_2$
$NaCoO_2$	α-$NaFeO_2$
$NaNiO_2$	α-$NaFeO_2$
$KInO_2$	α-$NaFeO_2$
$KTlO_2$	α-NaFeO
$RbInO_2$	α-$NaFeO_2$
$RbTlO_2$	α-$NaFeO_2$
$CsTlO_2$	α-$NaFeO_2$
$CuAlO_2$	α-$NaFeO_2$
$CuGaO_2$	α-$NaFeO_2$
$CuFeO_2$	α-$NaFeO_2$
$CuCoO_2$	α-$NaFeO_2$
$AgGaO_2$	α-$NaFeO_2$
$AgInO_2$	α-$NaFeO_2$
$AgTlO_2$	α-$NaFeO_2$
$AgCoO_2$	α-$NaFeO_2$
$AgNiO_2$	α-$NaFeO_2$
$AgNiSe_2$	α-$NaFeO_2$
$AgNiTe_2$	α-$NaFeO_2$
$NaAlSe_2$	TlSe
$NaAlTe_2$	TlSe
$NaGaTe_2$	TlSe
$NaInTe_2$	TlSe
$KAlTe_2$	TlSe
$KInTe_2$	TlSe
$CdTlSe_2$	TlSe
$LiInO_2$	α-$LiFeO_2$
$LiTlO_2$	α-$LiFeO_2$
$LiFeO_2$	α-$LiFeO_2$

Continuation of Table 3.5.1. Crystal Type, Space Group, and Number of Formula units (Z) are added for Selected Compounds.

Composition	Crystal type	Space group	Z
$NaNiSe_2$	NaCl	Fm3m	
$KAlSe_2$	$KAlSe_2$	P1	32
$KAlO_2$		Pbca	
$KGaS_2$		Aa	16
$KGaSe_2$		P1	32
KGaTe2		P1	32
$KGaO_2$		Pbca	16
$KInS_2$	$RbInS_2$	Cc	16
$KInSe_2$		P1	32
$KTlS_2$	$RbInS_2$	Cc	16
$KFeO_2$	$KFeO_2$	P2(1)nb	16
$KFeS_2$		C2/c	4
$KFeSe_2$		C2/c	4
$KCoO_2$		tetragonal	2
$RbGaO_2$	$KFeO_2$	P2(1)nb	16
$RbInS_2$	$RbInS_2$	Cc	16
$RbTlS_2$	$RbInS_2$	Cc	16
$RbFeS_2$		C2/c	4
$RbFeSe_2$		C2/c	4
$RbCoO_2$		Pbca	16
$CsAlO_2$		Fd3m	
$CsGaS_2$		C2/c	4
$CsInS_2$	$RbInS_2$	Cc	16
$CsTlS_2$	$RbInS_2$	Cc	16
$CsFeS_2$		Immm	4
$CsFeSe_2$		monoclinic	
$CuNiS_2$		cubic	
$AgAlO_2$		P6(3)/mmc	
$CdInS_2$	$CdTlS_2$	P3(-)m1	1
$CdTlS_2$	$CdTlS_2$	P3(-)m1	1
$HgTlS_2$		I4/mmm	8

Table 3.5.1.a. Pseudo-Binary Systems in which Compounds of Type ABX2 do not Form.

ZnS-TlS	without compound	AB_2Se_4
ZnO-FeO	without compound	AB_2Se_4
ZnO-CoO	without compound	AB_2Se_4
ZnO-NiO	without compound	AB_2Se_4
HgSe-TlSe	without compound	AB_2Se_4

3.5.1.2. Selection of Features.

On the basis of physical-chemical grounds two sets of chemical element features were selected for the description of oxide and chalcogenide compounds.

3.5.1.2.1. First Feature Set.

The first feature set coincides with Set I (see Section 3.4.2.1).

3.5.1.2.2.Set of Properties for Feature Set IV.

The set of properties of chemical elements for Feature Set IV includes the following information: the types of incomplete electronic shells of separate atoms, the isobaric thermal capacities at 298°K, the ionic radii, the first four ionization potentials, the electronegativities by Pauling, the energies of the crystal lattice, the temperatures and the heats of melting, the entropies of the individual substances at 298°K, Debye (characteristic) temperatures, and the formal valence of the elements A, B, or X represented in the compound of composition ABX_2. The quantitative properties were quantized on the basis of the uniform distribution of the interval values. Table 3.5.2 contains the gradations for Feature Set IV.

Table 3.5.2 Gradations for the Feature Set IV

Feature	Gradation	Feature	Gradation
Type of incomplete electronic shell			
s	Energy of the crystal lattice, S	Entropies at 298°K	
p	P	E*10 J/kg*mol	
d	D	[79-130]	E1
f	F	(130-182.8]	E2
		(182.8-244]	E3
Electronegative		(244-315.5]	E4
[0.7-0.8]	X1	(315.5-356.1]	E5
[0.8-1.09]	X2	(356.1-364.7]	E6
[1.09-1.2]	X3	(364.7-408]	E7
[1.2-1.3]	X4	(408-524]	E8
[1.3-1.5]	X5	(524-652]	E9
[1.5-1.7]	X6	(652-905]	E10
[1.7-1.8]	X7		
[1.8-2]	X8	Debye temp., K	
[2-2.2]	X9	[39.2-90]	TD1
[2.2-2.9]	X10	(90-129]	TD2
[2.9-4]	X11	(129-153]	TD3
		(153-163]	TD4
First Ionization potential, eV		(163-190]	TD5
		(190-233]	TD6
[3.893-5.39]	I11	(233-310]	TD7
[5.39-5.90]	I12	(310-405]	TD8
[5.90-6.31]	I13	(405-465]	TD9
[6.31-6.74]	I14	(465-585]	TD10
[6.74-6.95]	I15	(585-1860]	TD11
[6.95-7.432]	I16		
[7.432-7.87]	I17	Melting Point, K	
[7.87-8.64]	I18	[13.9-303]	TM1
[8.64-9.30]	I19	[303-527]	TM2
[9.30-10.55]	I110	[527-870]	TM3
[10.55-25]	I111	[870-1090]	TM4
		[1090-1323]	TM5
Second Ionization potential, eV		[1323-1629]	TM6
		[1629-1823]	TM7
[0-11.5]	I21	[1823-2473]	TM8
[11.5-12.4]	I22	[2473-3660]	TM9
[12.4-14.2]	I23		
[14.2-15.92]	I24	Heat of melting, kJ/mol	
[15.92-16.904]	I25	[0.1-2.2]	H1
[16.904-18.7]	I26	[2.2-4.6]	H2
[18.7-19.65]	I27		

Feature	Gradation	Feature	Gradation
[19.65-21.5]	I28	[4.6-8.3]	H3
[21.5-27.56]	I29	[8.3-10.9]	H4
[27.56-75.62]	I210	[10.9-13.8]	H5
		[13.8-15.7]	H6
Third Ionization potential, eV		[15.7-17.6]	H7
		[17.6-23.9]	H8
[0-21]	I31	[23.9-27.7]	H9
[21-24]	I32	[27.7-35.4]	H10
[24-25.61]	I33		
[25.61-29]	I34	Formal Valency	
[29-30.64]	I35	0	B0
[30.64-32.8]	I36	+1	B1
[32.8-34.21]	I37	+2	B2
[34.21-37]	I38	+3	B3
[37-47.426]	I39	+4	B4
[47.426-154]	I310	+5	B5
		+6	B6
Fourth Ionization potential, eV		+7	B7
		+8	B8
[0-36.7]	I41	-1	B1-
[36.7-41]	I42	-2	B2-
[41-44]	I43	-3	B3-
[44-46]	I44	-4	B4-
[46-48]	I45	-5	B5-
[48-52]	I46	-6	B6-
[52-56]	I47	-7	B7-
[56-64.2]	I48		
[97.16-259.3]	I410	capacity at 298°K kj/kg*mol*K	
Ionic radius, A			
[0-0.39]	R1	[7-20.808]	C1
(0.39-0.57]	R2	(20.808-23.41]	C2
(0.37-0.65]	R3	(23.41-24.79]	C3
[0.65-0.69]	R4	(24.79-25.246]	C4
[0.69-0.78]	R5	(25.246-26]	C5
[0.78-0.85]	R6	(26-26.377]	C6
[0.85-0.90]	R7	(26.377-27.18]	C7
[0.90-0.99]	R8	(27.18-28.01]	C8
[0.99-1.11]	R9	(28.01-31.359]	C9
[1.11-2.20]	R10	(31.359-95]	C10

3.5.1.3. Computer Learning.

Computer learning is carried-out for two learning sets in which the compounds from Table 3.5.1 were described in terms of the sets of the component properties I and IV. The system of concept formation CONFOR [14] was used for the computer learning and prediction. The pyramidal networks and the corresponding logical expressions were formed as a result of computer learning via CONFOR. Appendix 2 contains the logical expressions for various learning sets.

3.5.1.4. Predictions of Crystal Structure.

The table of predictions of crystal structure type for the compounds with composition ABX_2 (Table 3.5.3) comes from the comparison of the results of prediction with use of the descriptions in terms of Feature Sets I and IV (see Section 1.6.3). The following designations are used:

C - chalcopyrite
N - α-$NaFeO_2$
B - β-$NaFeO_2$
L - α-$LiFeO_2$
T - TlSe

- - the crystal structure differing from those listed above;
* - the compound of composition ABX_2 does not form.

Physical-chemical systems, have been investigated experimentally and used for computer learning. The analysis of Table 3.5.3 shows that few new compounds of the composition ABX_2 with the crystal structure ofchalcopyrite form at normal pressure. The most reliable predictions of the chalcopyrite structure were obtained for compounds of composition $HgFeSe_2$, $HgCoSe_2$, and $HgNiSe_2$. These predictions were obtained using two feature sets. At the same time the predictions of the structure type of chalcopyrite for compounds with composition $ZnGaSe_2$, $RbInTe_2$, $KTlTe_2$, $RbTlTe_2$, $CdTlTe_2$, $HgFeO_2$, $KFeTe_2$, $RbFeTe_2$, $HgCoO_2$, $CoCoS_2$, $KCoTe_2$, $RbCoTe_2$, and $HgNiO_2$ were obtained only for one feature set (the use of another set had given an unrecognized result). The analysis of Table 3.5.3 shows also that the volume of the learning set is too small for reliable prediction of new chalcopyrites of composition ABX_2.

3.5.2. Prediction of New Chalcopyrites w/Composition ABX_2 and CDY_2

Prediction of New Chalcopyrites of the Composition ABX_2 and CDY_2:

A = Mg, Ca, Sr, Ba, Zn, Cd, Hg; B = Si, Ge, Sn; X = N, P, As, Sb, Bi, S, Se, Te;
C = Li, Na, K, Rb, Cs; D = P, As, Sb, Bi; Y = N, P, As, Sb, Bi).

3.5.2.1. Data for Computer Learning.

The data for computer learning was extracted from the DB on ternary inorganic compound properties [18-21]. In this investigation we attempted to predict new compounds with composition given above which have the crystal structure resembling that of chalcopyrite (space group I4(-)2d) [35] and b-$NaFeO_2$ (space group $Pna2_1$) at normal pressure and room temperature.Table 3.5.4 contains a learning set.

Table 3.5.3 Crystal types of compounds with composition ABX_2

	B=Al				B=Ga				B=In				B=Tl				B=Fe				B=Co				B=Ni			
X	O	S	Se	Te	O	S	Se	Te	O	S	Se	Te	O	S	Se	Te	O	S	Se	Te	O	S	Se	Te	O	S	Se	Te
A																												
Li	N	B	0	0	B	0	0	0	L	0	B	C	L	0	0	0	L	0	0	0	0	0	0	0	N	0	0	0
Na	B*	0	T*	T*	B*	0	0	T*	N*	N*	N*	T*	N*	0	0	0	N*	0	0	0	N*	0	0	0	N*	T*	- *	T*
K	- *	0	- *	T*	- *	- *	- *	- *	N*	- *	- *	T*	N*	- *	0	C	- *	- *	- *	C	- *	-	C	0	0	0	0	0
Rb	- *	0	0	0	- *	0	0	0	N*	- *	0	C	N*	- *	0	C	-	- *	- *	C	- *	-	-	C	-	T	-	0
Cs	- *	0	0	0		- *	0	0	0	- *	0	0	N*	- *	0	0	-	- *	- *	0	- *	-	-	0	-	0	-	T
Cu	N*	C*	C*	C*	N*	C*	C*	C*	0	C*	C*	C*	0	C*	C*	C*	N*	C*	C*	C*	N*	C	0	0	N	- *	0	0
Ag	- *	C*	C*	C*	N*	C*	C*	C*	N*	C*	C*	C*	N*	0	C*	C*	C*	C*	C*	C*	N*	0	0	0	N*	N*	N*	N*
Au	0	0	0	0	0	0	0	0	0	-	0	0	0	0	0	0	L*	-	0	0	L*	-	-	0	L*	T	-	T
Zn	-	C*	C*	C*	-	-	C	C*	-	-	-	-	0	* *	0	C*	* *	-	0	0	* *	-	0	0	* *	-	0	
Cd	-	-	0	0	0	-	-	C*	T*	- *	-	0	0	- *	T*	C	T	-	0	0	T	-	0	0	T	-	0	0
Hg	0	0	0	-	0	-	0	C	C	0	0	-	0	-	*	0	C	0	C	0	C	0	C	0	C	0	C	0

Table 3.5.4 Learning set for Predicting Crystal Types with composition ABX_2

Composition	Crystal type
$MgSiP_2$	chalcopyrite
$ZnSiP_2$	chalcopyrite
$CdSiP_2$	chalcopyrite
$ZnSiAs_2$	chalcopyrite
$CdSiAs_2$	chalcopyrite
$ZnGeP_2$	chalcopyrite
$ZnGeAs_2$	chalcopyrite
$CdGeP_2$	chalcopyrite
$CdGeAs_2$	chalcopyrite
$CdGeTe_2$	chalcopyrite
$ZnSnP_2$	chalcopyrite
$ZnSnAs_2$	chalcopyrite
$ZnSnSb_2$	chalcopyrite
$CdSnP_2$	chalcopyrite
$CdSnAs_2$	chalcopyrite
$CaGeN_2$	chalcopyrite
$LiPN_2$	chalcopyrite
$MgSiN_2$	β $NaFeO_2$
$MgGeN_2$	β-$NaFeO_2$
$ZnGeN_2$	β-$NaFeO_2$

Composition	Crystal type	Space group	Z
$MgGeP_2$	ZnS		
$BaSnS_2$		$P2_(1)/c$	4
$NaPN_2$		I4(-)	4

Table 3.5.4.a. Ternary Systems in which ABX_2 does not Form

Cd-Sn-Sb	without compound AB_2Se_4
Cd-Sn-Bi	without compound AB_2Se_4
Cd-Sn-S	without compound AB_2Se_4
Cd-Sn-Se	without compound AB_2Se_4
Cd-Sn-Te	without compound AB_2Se_4
Hg-Sn-Bi	without compound AB_2Se_4
Hg-Sn-S	without compound AB_2Se_4
Hg-Sn-Se	without compound AB_2Se_4
Hg-Sn-Te	without compound AB_2Se_4
Mg-Si-Sb	without compound AB_2Se_4
Cd-Si-Te	without compound AB_2Se_4
Zn-Ge-Te	without compound AB_2Se_4
Cd-Ge-Se	without compound AB_2Se_4
Hg-Ge-S	without compound AB_2Se_4
Hg-Ge-Se	without compound AB_2Se_4
Hg-Ge-Te	without compound AB_2Se_4
Mg-Sn-Sb	without compound AB_2Se_4
Mg-Sn-Bi	without compound AB_2Se_4
Ca-Sn-S	without compound AB_2Se_4
Zn-Sn-Se	without compound AB_2Se_4
Zn-Sn-Te	without compound AB_2Se_4

On the basis of physical-chemical grounds two sets of chemical element features were selected. The first feature set coincides with Set I (see Section 3.4.2.1) but does not include the formal valence of elements, because it is difficult to determine one for compounds of this kind. The second feature set coincides with Set IV, but instead of ionic radii, covalent radii were included. See in Table 3.5.5 the gradations for the covalent radii. In addition, the formal valence of elements were excluded also.

Table 3.5.5 The gradations for covalent radii, A

Feature Value	Gradation Value
[0.28-0.66]	RC1
[0.66-0.77]	RC2
[0.77-1.00]	RC3
[1.00-1.14]	RC4
[1.14-1.22]	RC5
[1.22-1.27]	RC6
[1.27-1.33]	RC7
[1.33-1.40]	RC8
[1.40-1.54]	RC9

3.5.2.3.Computer Learning.

The computer learning is carried out for two learning sets in which the compounds from Table 3.5.4 were described in terms of the feature sets of the component properties I and IV with alterations. The system of concept

formation CONFOR [14] was used for the computer learning and predicting. Two pyramidal networks and the corresponding logical expressions were formed as a result of computer learning. Appendix 3 contains the logical expressions for various learning sets.

3.5.2.4. Predictions of Crystal Structure.
The tables of predictions of the crystal structure type for the compounds of the composition ABX_2 (Tables 3.5.6 and 3.5.7) result from the comparison of the results of prediction with descriptions in terms of Feature Sets I and IV (with alterations). See designations in Section 3.5.1.4.

The analysis of Table 3.5.6 and 3.5.7 shows that few new compounds of the composition ABX_2 with the crystal structure of the chalcopyrite form at normal pressure. We did not obtain the predictions of chalcopyrite structure using the two feature sets. The predictions of the chalcopyrite structure type for compounds with composition $MgGeAs_2$, $MgGeSb_2$, $CaGeAs_2$, $CaGeSb_2$, $CaSnBi_2$, $SrGeAs_2$, $SrGeSb_2$, $BaGeAs_2$, $BaGeSb_2$, $ZnSnN_2$, $HgGeAs_2$, $HgGeSb_2$, KPN_2, and $LiAsSb_2$, $NaAsSb_2$, $LiSbAs_2$, $NaSbAs_2$, $KSbAs_2$, and $KAsSb_2$, were obtained only for one feature set (the use of another set had given an unrecognized result). *These predictions are not reliable.* The analysis of these Tables shows also that the volume of the learning set is too small for reliable prediction of new chalcopyrites with composition ABX_2.

Table 3.5.6
Crystal types of compounds with composition ABX_2

	B=Si								B=Ge								B=Sn							
X	N	P	As	Sb	Bi	S	Se	Te	N	P	As	Sb	Bi	S	Se	Te	N	P	As	Sb	Bi	S	Se	Te
A																								
Mg	B*	C*	*	**	*	*	*	*	B*	-*	C	C	*	*	*	*			*	**	**	-*		
Ca	B	-	*	*		*	*	*	C*	-	C	C	*	*	*	*					C	**		
Sr			*	*		*	*	*	B	-	C	C	*	*	*	*			*	*		-*	*	
Ba			*	*		*	*	*	B	-	C	C	*	*	*	*			*	*	*	-*	*	*
Zn		C*	C*	*				*	B	C*	C*	B				**	C	C*	C*	C*			**	**
Cd		C*	C*	*	*	*	*	**		C*	C*	*	*	*	**	C*		C*	C*	**	**	**	**	**
Hg			**	**		*	*	**	B	-*	C*	C	*	**	**	**		**	**	**	**	**	**	**

Table 3.5.7
Crystal types of compounds with composition ABX_2

	B=P					B=As					B=Sb					B=Bi				
X	N	P	As	Sb	Bi	N	P	As	Sb	Bi	N	P	As	Sb	Bi	N	P	As	Sb	Bi
A																				
Li	C*	-				B			C		B		C							
Na	-*	-	-	-		B	-		C	*	B	-	C		*			*	*	
K	C	-	-	-		B	-		C	*	B	-	C		*			*	*	
Rb		-	-	-		B	-		B		B	-	B							
Cs		-	-	-		B	-		B		B	-	B		*				*	

CONCLUSIONS

1. The basic principles of prediction of inorganic compounds for new electro-optical, ferroelectric, superconducting, or semiconducting materials use computer learning strategies.

2. The ways for improvement of the reliability of prediction are based on the utilization of databases for the selection of learning examples, expert assessment of data for computer learning, and comparison of predictions which have been obtained using various feature sets.

3. The classes of the inorganic compounds exhibiting the most promise for searching for new electro-optical, ferro-electric, superconducting, and semiconducting materials are determined on the basis of analysis of the application domains and the known data.

4. Results of predicting the crystal structure types (chalcopyrite, Th_3P_4, $CaFe_2O_4$, Yb_3S_4, Yb_3Se_4, $PbGa_2Se_4$, $NiCr_2Se_4$, spinel, or olivine) at normal pressure and room temperature for compounds with composition AB_2Se_4 are presented.

5. Analysis of predictions showed that structures resembling olivine and $NiCr_2Se_4$ are an inherent feature of compounds with composition $A(IV)B(II)_2Se_4$, but the structure types Th_3P_4 and $NiCr_2Se_4$ are characteristic of compounds with composition $A(II)B(III)_2Se_4$.

6. Prediction of the crystal structure types (chalcopyrite, α- or β-$NaFeO_2$, α-$LiFeO_2$, or TlSe) at standard conditions for compounds with composition ABX_2 was carried-out. Analysis of the results shows also that the size of this learning set is too small for reliable prediction of new chalcopyrites of composition ABX_2.

[Added text by A. G. Jackson and S. R. LeClair:

In Summary, the objective of the above report was to report on initial efforts to develop a new approach, based on computer learning methods, for *a priori* prediction of inorganic compounds with predefined properties. Classes of compounds reported on include electro-optical, ferro-electric, superconducting and semiconducting materials. Families studied among these classes were chalcopyrites, spinels, and several A_xB_y and derivative type compounds. The above conclusions simply state that the predictions for AB_2Se_4 type compounds with Group IV and Group II cations suggest that chalcopyrite, spinel and Th_3P_4 structures do <u>not</u> occur and that olivine and $NiCr_2Se_4$ structures are strongly associated with AB_2Se_4 type compounds.

Furthermore, for AB_2Se_4 compounds with Group II and Group III cations, the predictions are that chalcopyrite and spinel structures also do <u>not</u> occur, but $NiCr_2Se_4$ structures and many Th_3P_4 compounds can be formed.

For the ABX_2 class of compounds, a few chalcopyrite structures were predicted, but an important considerstion regarding this result is that the training set was determined to be too small for reliable predictions.]

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Appendix 1

Appendix 1

[Added text by Drs LeClair and Jackson

The symbols listed below are indices of nodes corresponding to output from a pyramidal network. A graphical representation of this output is available via the software system CONFOR. Also available via CONFOR is the meaning of the node contents (attributes associated with the nodes), e.g. F314 represents a node. The symbol "*" represents the logical AND function and "V" represents the logical OR function. The collection of symbols, therefore, represent conjunction and disjunction of the attributes which taken together represent a concept.]

Logical Expressions for Predicting Crystal Types for Composition AB_2Se_4

Feature set I. Predicting the crystal type for Composition $A(IV)B(II)_2Se_4$

CONCEPT FOR CLASS chalcopyrite :

[1]
F414* D510* R6* P42* R2* S42* D310* P56* S62* D40* S50* P46* D410* S52* P50*S12* S22* P26* S32* P36* F40* D50* F50* S60* P60* D60* S70* B2* B4

CONCEPT FOR CLASS olivine :

[3]
S42* D40* S50* P50* S12* S22* P26* S32* P36* F40* D50* F50* S60* P60* D60*S70* B2* B4* P40*~{R2}*~{D32* R5}*~{D33* R3}*~{D310* P46* D410* S52* R3* P52*R4}
V [3]
P40* D30* S40*~{R2* S42* D310* P56* S62* D40* S50* P46* D410* S52* P50* S12*S22* P26* S32* P36* F40* D50* F50* S60* P60* D60* S70* B2* B4* R10* P32}
V [1]
S42* D310* D40* S50* P46* D410* S52* P50* S12* S22* P26* S32* P36* F40* D50*F50* S60* P60* D60* S70* B2* B4* P40* P52* R4* D30* S40* P30
V [1]
R2* S42* D40* S50* P50* S12* S22* P26* S32* P36* F40* D50* F50* S60* P60* D60*S70* B2* B4* P40* D30* S40* R10* P32*~{D310* P56* S62* P46* D410* S52}
V [1]
R2* S42* D40* S50* P50* S12* S22* P26* S32* P36* F40* D50* F50* S60* P60* D60*S70* B2* B4* P40* D30* S40* P32* D35

CONCEPT FOR CLASS $NiCr_2S_4$:

[17]
D40* S50* P50* S12* S22* P26* S32* P36* F40* D50* F50* S60* P60* D60* S70* B2*B4* P40*~{S42}*~{S42* D310* P46* D410* S52* R3* P52* R4}*~{P42* R2* S42* D310*R3}
V [11]
R2* S42* D40* S50* P50* S12* S22* P26* S32* P36* F40* D50* F50* S60* P60*

D60*S70* B2* B4* P40*~{D30* S40* P32* D35}*~{D30* S40* R10* P32}*~{D310* P56* S62*P46* D410* S52* D30* S40* R10* P32}*~{P42* D310* R3}
V [9]
S42* D40* S50* P50* S12* S22* P26* S32* P36* F40* D50* F50* S60* P60* D60*S70* B2* B4* P40* D32* R5
V [6]
S42* D40* S50* P50* S12* S22* P26* S32* P36* F40* D50* F50* S60* P60* D60*S70* B2* B4* P40* D33* R3

CONCEPT FOR CLASS another_structure :

[6]
S42*~{R2* D40* S50* P50* S12* S22* P26* S32* P36* F40* D50* F50* S60* P60*D60* S70* B2* B4* P40}*~{D40* S50* P50* S12* S22* P26* S32* P36* F40* D50*F50* S60* P60* D60* S70* B2* B4* P40* D32* R5}*~{D40* S50* P50* S12* S22* P26*S32* P36* F40* D50* F50* S60* P60* D60* S70* B2* B4* P40* D33* R3}*~{D310*P46* D410* S52* S12* S22* P26* S32* P36* F40* D50* F50* S60* P60* D60* S70*B2* B4* P52* R4}*~{D40* S50* P50* S12* S22* P26* S32* P36* F40* D50* F50* S60*P60* D60* S70* B2* B4* P40}*~{F414* D510* R6* P42* R2* D310* P56* S62* D40*S50* P46* D410* S52* P50* S12* S22* P26* S32* P36* F40* D50* F50* S60* P60*D60* S70* B2* B4}*~{D310* D40* S50* P46* D410* S52* P50* S12* S22* P26* S32*P36* F40* D50* F50* S60* P60* D60* S70* B2* B4* P40* R3* P52* R4}*~{D310* D40*S50* P46* D410* S52* P50* S12* S22* P26* S32* P36* F40* D50* F50* S60* P60*D60* S70* B2* B4* P40* P52* R4* D30* S40* P30}*~{R2* D40* S50* P50* S12* S22*P26* S32* P36* F40* D50* F50* S60* P60* D60* S70* B2* B4* P40* D30* S40* P32*D35}*~{R2* D40* S50* P50* S12* S22* P26* S32* P36* F40* D50* F50* S60* P60*D60* S70* B2* B4* P40* D30* S40* R10* P32}
V [6]
D310*~{S42* P46* D410* S52* S12* S22* P26* S32* P36* F40* D50* F50* S60* P60*D60* S70* B2* B4* P52* R4}*~{F414* D510* R6* P42* R2* S42* P56* S62* D40* S50*P46* D410* S52* P50* S12* S22* P26* S32* P36* F40* D50* F50* S60* P60* D60*S70* B2* B4}*~{S42* D40* S50* P46* D410* S52* P50* S12* S22* P26* S32* P36*F40* D50* F50* S60* P60* D60* S70* B2* B4* P40* R3* P52* R4}*~{S42* D40* S50*P46* D410* S52* P50* S12* S22* P26* S32* P36* F40* D50* F50* S60* P60* D60*S70* B2* B4* P40* P52* R4* D30* S40* P30}
V [6]
S12* S22* P26* S32* P36* F40* D50* F50* S60* P60* D60* S70* B2* B4*~{D40* S50*P50* P40}*~{R2* S42* D40* S50* P50* P40}*~{S42* D40* S50* P50* P40* D32* R5}*~{S42* D40* S50* P50* P40* D33* R3}*~{S42* D310* P46* D410* S52* P52* R4}*~{S42* D40* S50* P50* P40}*~{F414* D510* R6* P42* R2* S42* D310* P56* S62*D40* S50* P46* D410* S52* P50}*~{S42* D310* D40* S50* P46* D410* S52* P50*P40* R3* P52* R4}*~{S42* D310* D40* S50* P46* D410* S52* P50* P40* P52* R4*D30* S40* P30}*~{R2* S42* D40* S50* P50* P40* D30* S40* P32* D35}*~{R2* S42*D40* S50* P50* P40* D30* S40* R10* P32}
V [1]
R2* S42* D310* P56* S62* D40* S50* P46* D410* S52* P50* S12* S22* P26* S32*P36* F40* D50* F50* S60* P60* D60* S70* B2* B4* P40* D30* S40* R10* P32
V [1]
P42* R2* S42* D310* D40* S50* P50* S12* S22* P26* S32* P36* F40* D50* F50*S60* P60* D60* S70* B2* B4* P40* R3
V [1]
F414* D510* R6* S42* D310* P56* S62* P46* D410* S52* S12* S22* P26* S32* P36*F40* D50* F50* S60* P60* D60* S70* B2* B4* P52* R4

CONCEPT FOR CLASS without_Compound_AB_2Se_4 :

[4]

S42* D310* P46* D410* S52* S12* S22* P26* S32* P36* F40* D50* F50* S60* P60*D60* S70* B2* B4* P52* R4*~{D40* S50* P50* P40* D30* S40* P30}*~{F414* D510*R6* P56* S62}

V [1]

S42* D310* D40* S50* P46* D410* S52* P50* S12* S22* P26* S32* P36* F40* D50*F50* S60* P60* D60* S70* B2* B4* P40* R3* P52* R4

Feature Set I. Predicting Crystal Type for Composition $A(II)B(III)_2Se_4$

CONCEPT FOR CLASS chalcopyrite :

[6]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60*B3*P36*~{D410*P46* S52}*~{S41}*~{P42* P50* D40* S50}*~{P46* S52* P50* D40* S50*R10* P31* D30* R2* S40* P40}*~{P46* S52* P50* D40* S50* R10* P40* D33* R3}*~{P50* D40* S50* R2* P40* D36* P41}*~{P50* D40* S50* R2* P40* R3* D35}*~{P50* D40* S50* R10* D30* R2* P40* P41}*~{P46* P50* D40* S50* R2* P40* R3* D37*D48* S51}*~{P46* P50* D40* S50* R2* P40* R3* D48* S51* D38}*~{P46* S52* P50*D40* S50* R10* D30* P40* D41* R8}*~{P46* S52* P50* D40* R10* D41* R8}*~{P50*D40* S50* R2* P40* P41* D35}*~{P50* D40* S50* R2* P40* D35* P43}

V [6]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*~{S60*F40* P50}*~{S60* F40* D410* P46* S52}*~{D410* P46* S52* S62* P56}

V [2]
S60* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* P50*D40* S50* P40* R3*~{D33}*~{S41* D35}*~{D310* P46}*~{D310* R2* D35}

V [2]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P50* D40* S50* P40* R3*~{P46}*~{D35}*~{R2* D35}*~{P46* R2* D37* D48* S51}*~{P46* R2* D48* S51* D38}*~{D410* P46* S52* S41* D35* P51* R5}*~{P46* S41* R2*D48* S51}

V [2]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P50* D40* S50* R2* P41*~{D410* P46* S52* S62* P56}*~{P40* D36}*~{R10* D30*P40}*~{P40* D35}*~{D410* P46* S52* P52* R4}*~{P42}*~{S41* P40}

V [2]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* P51* R5*~{}

V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P50* D40* S50* P31* D30* R2* S40* P40* R3

V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* P40* R3* P51* R5*~{S41* D35}

V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* R2* P41* R5

V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* R2* P41* S62* P56* R6* D510* F414

V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* S62* P56* P51* R5* R6* D510* F414

CONCEPT FOR CLASS spinel :

[13]
D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*~{R8}*~{D310*

S42*D410* P46* S52* S62* P56}*~{S60* F40* S42* P50* D40* S50* P40* R5*
D32}*~{D310* S42}*~{S60* F40* S42* P50* D40* S50* P40* D33* R3}*~{S60*
F40* S42* P50*D40* S50* R2* P40* D36}*~{S60* D310* F40* S42* P46* S52*
P50* D40* S50* P40}*~{S60* F40* S41* P50* D40* S50* P40* R3* D35}*~{D30*
S40}*~{S60* D310* F40*S42* P46* S52* P50* D40* S50* R10*
P40}*~{F42}*~{S60* F40* S42* P50* D40* S50*R2* P40* D35* R5* D32}*~{S60*
F40* S42* P50* D40* S50* R2* P40* D38* R5* D32}*~{S60* F40* S42* P50* D40*
S50* R2* P40* D33* R3* D35}*~{S60* F40* S42* P50*D40* S50* R2* P40* D33*
R3* D38}*~{S60* F40* S42* S41* P50* D40* S50* R2* P40*R3* D35* D38}
V [13]
S60* F40* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*~{S42}*~{R3}*~{D310}
V [13]
S60* F40* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*~{P50* D40*
S50*P40}*~{D310* S42* P36* D410* P46* S52* S62* P56}*~{D310* S42* P36}
V [13]
P50*~{D40* S50}*~{S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60*
S70*B2* P60* B3* P36}
V [11]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*P50*~{D40* S50}*~{D410* P46* S52* S62* P56}*~{D40* S50* P40}*~{D410*
P46* S52*P51* R5}*~{P46* S52* D40* R10* D41* R8}
V [6]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52*~{P50* D40* S50}*~{S62* P56} {P50* S62*
P56}*~{R4}*~{P50* D40*S50* R2}*~{P50* P51* R5}
V [5]
S60* D310* F40* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
S41*~{S42* P50* D40* S50* R2* P40}*~{S42* D410* P46* S52* P50* D40* S50*
P40*P51* R5}*~{S42* P46* P50* D40* S50* P40* R3* D35}*~{S42* P46* P50*
D40* S50*P40* R3* D35* D48* S51}
V [4]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*S41*~{P50* D40* S50* R2* P40}*~{D410* P46* S52* P50* D40* S50* P40*
P51* R5}*~{P46* P50* D40* S50* P40* R3* D35}*~{P46* P50* D40* S50* P40*
R3* D35* D48*S51}
V [4]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*P50* D40* S50* R2* P40*~{}*~{P46* S52}*~{P46* S52* R10* P31* D30*
S40}*~{R10*D30* P41}*~{P46* R3* D37* D48* S51}*~{P46* R3* D48* S51*
D38}*~{P41* D35}*~{D35* P43}*~{D410* P46* S52* R10* P31* D30* S40* S62*
P56}*~{D410* P46* S52*D35* R8* S62* P56* D510* F414* P63}
V [4]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* S62* P56* R5*~{R8* F47* D51}*~{D51* R9}*~{D510*
F414*P61* R7}
V [3]
S60* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
P50*D40* S50* R2* P40* D35*~{D310* P41}*~{D310* P43}*~{R5* D32}*~{D33*
R3}*~{S41*R3* D38}*~{D310* D410* P46* S52* R8* S62* P56* D510* F414* P63}
V [3]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*P50* D40* S50* P40* R3* D35*~{P46* S41}*~{P46* S41* D48* S51}
V [2]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*S41* P50* D40* S50* P40* R3* D35*~{P46}*~{P46* D48* S51}

V [2]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* R8* R5*~{S62* P56* F47* D51}

V [1]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P50* D40* S50* R2* P40* D36* P41

V [1]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P50* D40* S50* R2* P40* R3* D35

V [1]

S60* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* P50*D40* S50* R2* P40* D35* R7* D31

V [1]

S60* D310* F40* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* S41*P50* D40* S50* R2* P40* R3* D35

V [1]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* S41* P50* D40* S50* P40* R3* D35* S62* P56* R6* D510* F414

V [1]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*S41* P50* D40* S50* R2* P40* D35

V [1]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P46* S41* P50* D40* S50* R2* P40* R3* D48* S51

V [1]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D41* R8* R5

V [1]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* R8* S62* P56* R5* F410

V [1]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* S62* P56* R5* R7* F413

V [1]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* R10* S62* P56* R5* F414

V [1]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* S62* P56* R5* F414* D51* R7

CONCEPT FOR CLASS $PbGa_2Se_4$:

[11]

S60* D310* F40* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*~{S42}*~{S42* P50}*~{S41}*~{S42* P50* D40* S50* P31* D30* R2* S40* P40* R3}*~{S42* P50* D40* S50* R2* P40* R3* D35}*~{S42* P46* P50* D40* S50* R2* P40* R3*D37* D48* S51}*~{S42* P46* P50* D40* S50* R2* P40* R3* D48* S51* D38}*~{S42*P46* S41* P50* D40* S50* R2* P40* R3* D48* S51}

V [11]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*~{}*~{P50}*~{D410* P46* S52* S62* P56* R6* D510* F414}*~{D410* P46*

S52* S62*P56* P51* R5* R6* D510* F414}*~{D410* P46* S52* S41* P50* D40* S50* P40* R3*D35* S62* P56* R6* D510* F414}

V [9]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* S62* P56*~{D510* F414}*~{R8* D510* F414* P63}*~{P50* D40* S50*R10* D30* P40* F414}*~{R10* R4* P53}*~{P50* D40* S50* R10* P31* D30* R2* S40*P40}*~{P50* R8* R5* F410}*~{P50* R5* R7* F413}*~{P50* R10* R5* F414}*~{P50*R8* R5* F47* D51}*~{P50* R5* D51* R9}*~{P50* R5* F414* D51* R7}*~{S41* P50*D40* S50* P40* R3* D35* D51* R9}*~{S41* P50* D40* S50* P40* R3* D35* F42* R9}*~{S41* P50* D40* S50* P40* R3* D35* R8* F44}*~{S41* P50* D40* S50* P40* R3*D35* R8* F46}*~{S41* P50* D40* S50* R10* P40* R3* D35* F47}*~{P50* D40* S50*R10* D30* P40* R8* F411}*~{P50* D40* S50* R10* D30* P40* R8* F410}*~{P50* D40*S50* R10* P40* F47* R7* D31}*~{P50* D40* R10* R8* D51* F48}*~{P50* D40* R10*R8* F411}*~{P50* D40* R10* R7* F412}*~{P50* D40* R10* R7* F413}*~{P50* D40* -R10* F414* D51* R7}*~{P50* R10* D41* R8}*~{P50* D40* S50* R10* P40* D33* R3* F47}*~{S41* P50* D40* S50* R10* P40* R3* D35}*~{S41* P50* D40* S50* P40* R3*D35* R8* D51* F48}*~{S41* P50* D40* S50* P40* R3* D35* F414* D51* R7}*~{P42*P50* D40* S50* R10* R2* F47}*~{P42* P50* D40* S50* R10* R2* F414}*~{R8* P52*R4* F44}*~{S41* P50* D40* S50* R2* P40* R8* F44}*~{S41* P50* D40* S50* R2*P40* R8* F47* D51}*~{P50* D40* S50* R2* R8* P43* F46}

V [9]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*P36* D410* P46* S52* S62* P56*~{}*~{P50}

V [9]

D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* D410*P46* S52* S62* P56*~{S60* F40}*~{R8* F46}*~{R10* F414}*~{F40* R10* R8* F410}*~{D510* F414* F42* R9* R7* P62}*~{R8* D510* F414* R7* P62* F43}*~{F40* R10*F47* D51* R9}*~{R10* R8* F47* F43}*~{R10* R8* F47* F44}*~{R10* R8* F47* D51*F48}*~{R10* R8* F47* F411}*~{R10* F47* R7* F412}*~{R10* F47* R7* F413}*~{D510* F414* R7* F412* P62}

V [9]

D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* D410*P46* S52* S62* P56*~{F40* R10}*~{S60* F40* P50}*~{R8}*~{R10* F47}*~{F40* D51}*~{S60* F40* D510* F414}*~{R10* F414}*~{D510* F414* R7* P62}*~{S60* F40* P50*D51}*~{S60* F40* P50* R8* R5* F47* D51}*~{S60* F40* P50* R5* D51* R9}*~{S60*F40* P50* R5* F414* D51* R7}

V [8]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P50* D40* S50*~{P46* S52}*~{P42}*~{S41* P40* R3* D35}*~{P31* D30* R2* S40*P40* R3}*~{R2* P40* D36* P41}*~{R2* P40* R3* D35}*~{P46* R2* P40* R3* D37*D48* S51}*~{P46* R2* P40* R3* D48* S51* D38}*~{R2* P40* P41* D35}*~{R2* P40*D35* P43}*~{P46* S41* R2* P40* R3* D48* S51}*~{S41* R2* P40* P41}*~{S41* R2*P40* D35}

V [6]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* S62* P56*~{}*~{P40}*~{R10* P40}*~{R10* D30*P40* F414}*~{R10* P31* D30* R2* S40* P40}*~{S41* R10* P40* R3* D35* F47}*~{R10* D30* P40* R8* F411}*~{R10* D30* P40* R8* F410}*~{R10* P40* F47* R7* D31}*~{R10* P40* D33* R3* F47}*~{R10* D30* P40* R8}

V [4]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P46* S52* P50* D40* S50* D30* S40* P40*~{D410* R10* P31* R2* S62* P56}*~{D410* P51* R5* R4* P30}

V [4]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P46* S52* P50* D40* S50* P40*~{D410}*~{D410* S62* P56}*~{R10* D33* R3}*~{S41*R10* R3* D35}*~{R10* D30* D41* R8}*~{D410* R10* P31* D30* R2* S40* S62* P56}

V [4]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P46* S52* P50* D40* S50* P40*~{D410}*~{D410* S62* P56}*~{D410* R10* S62* P56}*~{R10* D33* R3}*~{R10}*~{D410* R10* D30* S62* P56* F414}*~{S41* R10* R3* D35}*~{R10* D30* D41* R8}*~{D410* R10* P31* D30* R2* S40* S62* P56}*~{D410* S41*R10* R3* D35* S62* P56* F47}*~{D410* R10* D30* R8* S62* P56* F411}*~{D410*R10* D30* R8* S62* P56* F410}*~{D410* R10* S62* P56* F47* R7* D31}*~{D410*R10* D33* R3* S62* P56* F47}*~{D410* R10* D30* R8* S62* P56}*~{D410* D30* S40*P51* R5* R4* P30}*~{D410* R10* D30* P51* R5}

V [3]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P46* S52* P50* D40* S50* R10* P31* D30* R2* S40* P40*~{D410* S62* P56}

V [3]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* R2* P41* S62* P56*~{R6* D510* F414}

V [3]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* S62* P56* P51* R5*~{R6* D510* F414}

V [2]
S60* D310* F40* S42* D50* S12* S22* P26*S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* R10* R2* P41* S62* P56

V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P50* D40* S50* R10* D30* R2* P40* P41

V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* R10* P31* D30* R2* S40* P40* S62* P56* F47

V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* R10* P31* D30* R2* S40* P40* S62* P56* F414

V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* P31* D30* R2* S40* P40* S62* P56* D510* F414* R7* P62

V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* R10* R2* P41* S62* P56* F47

V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* R2* P41* S62* P56* D510* F414* R7* P62

V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* R8* S62* P56* P51* R5* F46

V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* R10* S62* P56* P51* R5* F47

V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* R10* S62* P56* P51* R5* F414

CONCEPT FOR CLASS $NiCr_2S_4$:

[18]
S60* F40* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P50* D40* S50*P40*~{P36* R10}*~{D310* S42* P36}*~{D310* S42* P36* D410* P46* S52* S41* R3*D35* S62* P56}*~{D310* S42* P36* P46* S52}*~{D310* S42* P36* P46* S52* R10*D33* R3}*~{D310* S42* P36* S41* R3* D35}*~{D310* S42* P36* P46* S52* S41* R10*R3* D35}*~{R4* P30}*~{D310* S42* P36* R2* D36* P41}*~{D310* S42* P36* D410*P46* S52* S41* R3* D35* P51* R5}*~{S42* P36* R2* D35* R7* D31}*~{D310* P36*S41* R2* R3* D35}
V [17]
S60* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* P50*D40* S50* P40*~{D310}*~{R2}*~{R3}*~{R5}
V [12]
S60* F40* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* R3*~{D310* S42* P46* P50* D40* S50* P40}*~{D310* S42* D410* P46* S52* S41* P50*D40* S50* P40* D35* S62* P56}*~{D310* S42* P46* S52* P50* D40* S50* R10* P40*D33}*~{D310* S42* S41* P50* D40* S50* P40* D35}*~{D310* S42* P46* S52* S41*P50* D40* S50* R10* P40* D35}*~{D310* S42* P50* D40* S50* P31* D30* R2* S40*P40}*~{D310* S42* P50* D40* S50* R2* P40* D35}*~{D310* S42* D410* P46* S52*S41* P50* D40* S50* P40* D35* P51* R5}*~{D310* S41* P50* D40* S50* R2* P40*D35}
V [7]
S60* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* P50*D40* S50* P40* R5* D32
V [6]
S60* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* P50*D40* S50* P40* D33* R3*~{D310* P46* S52* R10}
V [5]
S60* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* P50*D40* S50* R2* P40* D36*~{D310* P41}
V [4]
S60* F40* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* S41* P50*D40* S50* P40* R3* D35*~{D310* S42* D410* P46* S52* S62* P56}*~{D310* S42}*~{D310* S42* P46* S52* R10}*~{D310* S42* D410* P46* S52* P51* R5}*~{D310* R2}
V [3]
S60* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* S41*P50* D40* S50* P40* R3* D35*~{D310* D410* P46* S52* S62* P56}*~{D310}*~{D310*P46* S52* R10}*~{D310* D410* P46* S52* P51* R5}
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P46* S41* P50* D40* S50* P40* R3* D35* D48* S51
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P46* S41* P50* D40* S50* P40* R3* D35*~{D410* S52* S62* P56}*~{S52* R10}*~{D410* S52* P51* R5}
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P46* P50* D40* S50* R2* P40* R3* D37* D48* S51

V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P46* P50* D40* S50* R2* P40* R3* D48* S51* D38

V [1]
S60* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* P50*D40* S50* R2* P40* D35* R5* D32

V [1]
S60* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* P50*D40* S50* R2* P40* D38* R5* D32

V [1]
S60* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* P50*D40* S50* R2* P40* D33* R3* D35

V [1]
S60* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* P50*D40* S50* R2* P40* D33* R3* D38

V [1]
S60* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* S41*P50* D40* S50* R2* P40* R3* D35* D38

.CONCEPT FOR CLASS Th_3P_4 :

[18]
D310* S42* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* D410* P46*S52* S62* P56*~{S60* F40* D50}*~{D51}*~{D50}*~{S60* F40* D50* P50* D40* S50*R10* P40}*~{S60* F40* D50* P50* D40* S50* R2* P40}*~{R8* D510* F414* P63}*~{S60* F40* D50* P50* D40* S50* R10* D30* P40* F414}*~{S60* F40* D50* P50* D40*S50* P40* R3* D51}*~{S60* F40* D50* S41* P50* D40* S50* P40* R3* D35* R6*
D510* F414}*~{S60* F40* D50* P50* D40* S50* R10* D30* P40* R8* F411}*~{S60*F40* D50* P50* D40* S50* R10* D30* P40* R8* F410}*~{S60* F40* D50* P50* D40*S50* R10* P40* F47* R7* D31}*~{S60* F40* D50* P50* D40* S50* R10* P40* D33*R3* F47}*~{S60* F40* D50* S41* P50* D40* S50* R10* P40* R3* D35}*~{S60* F40*D50* S41* P50* D40* S50* P40* R3* D35* D510* F414* R7* P62}*~{S60* F40* D50*P50* D40* S50* P40* R3* R8* D510* F414* P63}

V [11]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* D410*P46* S52* R8* S62* P56*~{R10* F414}*~{F40* D510* F414* P63}*~{S60* F40* P50*D40* S50* R2* P40* D35* D510* F414* P63}*~{S60* F40}*~{S60* F40* P51* R5* F46}*~{S60* F40* P50* R10* D41}*~{S60* F40* S41* P50* D40* S50* P40* R3* D35* D51*F48}*~{S60* F40* P50* D40* S50* R2* P43* F46}*~{F40* R10}*~{R10* F47}*~{F40*R10* F46}

V [11]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* D410*P46* S52* R8* S62* P56*~{}*~{F47* D51}*~{S60* F40* P51* R5* F46}*~{S60* F40*P50* D40* S50* R2* P43* F46}*~{R10* F47}*~{F40* R10* F46}

V [11]
D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* R8*~{D310* S42*D410* P46* S52* S62* P56}*~{D310* S42}*~{D310* S42* D410* P46* S52* S62* P56*F47* D51}*~{S60* D310* F40* S42* D410* P46* S52* S62* P56* P51* R5* F46}*~{S60* D310* F40* S42* D410* P46* S52* P50* D40* S50* R2* P43* S62* P56* F46}*~{D310* S42* D410* P46* S52* R10* S62* P56* F47}*~{D310* F40* S42* D410* P46*S52* R10* S62* P56* F46}

V [7]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*

P36*D410* P46* S52* P50* S62* P56*~{D40* S50* R2}*~{D40* S50* R10* D30*
P40* F414}*~{S41* D40* S50* P40* R3* D35* R6* D510* F414}*~{R8* R5*
F410}*~{R5* R7*F413}*~{R10* R5* F414}*~{R5* F414* D51* R7}*~{R5* D510*
F414* P61* R7}*~{D40*S50* R10* D30* P40* R8* F411}*~{D40* S50* R10* D30*
P40* R8* F410}*~{D40* S50*R10* P40* F47* R7* D31}*~{D40* R10* R8* D51*
F48}*~{D40* R10* R8* F411}*~{D40* R10* R7* F412}*~{D40* R10* R7*
F413}*~{D40* R10* F414* D51* R7}*~{R10*D41* R8}*~{D40* S50* R10* P40*
D33* R3* F47}*~{S41* D40* S50* R10* P40* R3*D35}*~{S41* D40* S50* P40*
R3* D35* R8* D51* F48}*~{S41* D40* S50* P40* R3*D35* F414* D51*
R7}*~{S41* D40* S50* P40* R3* D35* D510* F414* R7* P62}*~{D40* S50* P40*
R3* R8* D510* F414* P63}
V [7]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* S62* P56*~{D40* S50* R2}*~{D40* S50* R10* D30*
P40* F414}*~{P42* D40* S50* R10* R2}*~{S41* D40* S50* P40* R3* D35* R6*
D510* F414}*~{R8* R5* F410}*~{R5* R7* F413}*~{R10* R5* F414}*~{R5* F414*
D51* R7}*~{R5*
D510* F414* P61* R7}*~{D40* S50* R10* D30* P40* R8* F411}*~{D40* S50*
R10*D30* P40* R8* F410}*~{D40* S50* R10* P40* F47* R7* D31}*~{D40* R10*
R8* D51*F48}*~{D40* R10* R8* F411}*~{D40* R10* R7* F412}*~{D40* R10* R7*
F413}*~{D40*R10* F414* D51* R7}*~{R10* D41* R8}*~{D40* S50* R10* P40*
D33* R3* F47}*~{S41* D40* S50* R10* P40* R3* D35}*~{S41* D40* S50* P40*
R3* D35* R8* D51* F48}*~{S41* D40* S50* P40* R3* D35* F414* D51*
R7}*~{S41* D40* S50* P40* R3* D35*D510* F414* R7* P62}*~{D40* S50* P40*
R3* R8* D510* F414* P63}
V [7]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* S62* P56*~{D40* S50* R2}*~{D40* S50* R10* D30*
P40* F414}*~{S41* D40* S50* P40* R3* D35* R6* D510* F414}*~{R8* R5*
F410}*~{R5* R7*F413}*~{R10* R5* F414}*~{R5* F414* D51* R7}*~{R5* D510*
F414* P61* R7}*~{D40*S50* R10* D30* P40* R8* F411}*~{D40* S50* R10* D30*
P40* R8* F410}*~{D40* S50*R10* P40* F47* R7* D31}*~{D40* R10* R8* D51*
F48}*~{D40* R10* R8* F411}*~{D40* R10* R7* F412}*~{D40* R10* R7*
F413}*~{D40* R10* F414* D51* R7}*~{R10*D41* R8}*~{D40* S50* R10* P40*
D33* R3* F47}*~{S41* D40* S50* R10* P40* R3*D35}*~{S41* D40* S50* P40*
R3* D35* R8* D51* F48}*~{S41* D40* S50* P40* R3*D35* F414* D51*
R7}*~{S41* D40* S50* P40* R3* D35* D510* F414* R7* P62}*~{D40* S50* P40*
R3* R8* D510* F414* P63}
V [7]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* S62* P56*~{D40* S50}*~{D40* S50*
R2}*~{R10}*~{D40* R10}*~{D40* S50* R2* P40}*~{D51}*~{D40* S50* R10* D30*
P40* F414}*~{D40* S50* P40*R3* D51}*~{S41* D40* S50* P40* R3* D35* R6*
D510* F414}*~{R8* R5* F410}*~{R5*R7* F413}*~{R10* R5* F414}*~{R5* F414*
D51* R7}*~{R5* D510* F414* P61* R7}*~{D40* S50* R10* D30* P40* R8*
F411}*~{D40* S50* R10* D30* P40* R8* F410}*~{D40* S50* R10* P40* F47* R7*
D31}*~{D40* R10* R8* D51* F48}*~{D40* R10* R8*F411}*~{D40* R10* R7*
F412}*~{D40* R10* R7* F413}*~{D40* R10* F414* D51* R7}*~{R10* D41*
R8}*~{D40* S50* R10* P40* D33* R3* F47}*~{S41* D40* S50* R10*P40* R3*
D35}*~{S41* D40* S50* P40* R3* D35* R8* D51* F48}*~{S41* D40* S50*P40*
R3* D35* F414* D51* R7}*~{S41* D40* S50* P40* R3* D35* D510* F414*
R7*P62}*~{D40* S50* P40* R3* R8* D510* F414* P63}
V [7]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*

P36*P50*~{P46* S52}*~{}*~{R10}*~{D410* P46* S52* D40* S50* S62*
P56}*~{D410* P46*S52* D40* S50* S62* P56}*~{P46* S52* D40* S50* R2*
P40}*~{D410* P46* S52* D40*S50* R2* S62* P56}*~{D410* P46* S52*
R5}*~{D410* P46* S52* R10* S62* P56}*~{D410* P46* S52* D40* R10* S62*
P56}*~{P46* D40* S50* P40* R3}*~{D410* P46*S52* D40* S50* R2* P40* S62*
P56}*~{D410* P46* S52* S62* P56* D51}*~{D410*P46* S52* D40* S50* R10*
D30* P40* S62* P56* F414}*~{D410* P46* S52* D40* S50*P40* R3* S62* P56*
D51}*~{P46* S41* D40* S50* P40* R3* D35}*~{D410* P46* S52*
S41* D40* S50* P40* R3* D35* S62* P56* R6* D510* F414}*~{P46* S41* D40*
S50*P40* R3* D35* D48* S51}*~{D410* P46* S52* R8* S62* P56* R5*
F410}*~{D410* P46*S52* S62* P56* R5* R7* F413}*~{D410* P46* S52* R10*
S62* P56* R5* F414}*~{D410* P46* S52* S62* P56* R5* F414* D51* R7}*~{D410*
P46* S52* S62* P56* R5*D510* F414* P61* R7}*~{D410* P46* S52* D40* S50*
R10* D30* P40* R8* S62* P56*F411}*~{D410* P46* S52* D40* S50* R10* D30*
P40* R8* S62* P56* F410}*~{D410*P46* S52* D40* S50* R10* P40* S62* P56*
F47* R7* D31}*~{D410* P46* S52* D40*R10* R8* S62* P56* D51* F48}*~{D410*
P46* S52* D40* R10* R8* S62* P56* F411}
~{D410 P46* S52* D40* R10* S62* P56* R7* F412}*~{D410* P46* S52* D40*
R10*S62* P56* R7* F413}*~{D410* P46* S52* D40* R10* S62* P56* F414* D51*
R7}*~{D410* P46* S52* R10* D41* R8* S62* P56}*~{D410* P46* S52* D40* S50*
R10* P40*D33* R3* S62* P56* F47}*~{D410* P46* S52* S41* D40* S50* R10*
P40* R3* D35*S62* P56}*~{D410* P46* S52* S41* D40* S50* P40* R3* D35* R8*
S62* P56* D51*F48}*~{D410* P46* S52* S41* D40* S50* P40* R3* D35* S62*
P56* F414* D51* R7}*~{D410* P46* S52* S41* D40* S50* P40* R3* D35* S62*
P56* D510* F414* R7* P62}*~{D410* P46* S52* D40* S50* P40* K[illegible] R8* S62*
P56* D510* F414* P63}
V [7]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*P50*~{P46* S52}*~{}*~{D410* P46* S52* D40* S50* S62* P56}*~{D410* P46*
S52*D40* S50* R2* S62* P56}*~{D410* P46* S52* R10* S62* P56}*~{D410* P46*
S52*D40* R10* S62* P56}*~{P46* D40* S50* P40* R3}*~{D410* P46* S52* D40*
S50* R2*P40* S62* P56}*~{D410* P46* S52* S62* P56* D51}*~{D410* P46* S52*
D40* S50*R10* D30* P40* S62* P56* F414}*~{D410* P46* S52* D40* S50* P40*
R3* S62* P56*D51}*~{P46* S41* D40* S50* P40* R3* D35}*~{D410* P46* S52*
S41* D40* S50* P40*R3* D35* S62* P56* R6* D510* F414}*~{P46* S41* D40*
S50* P40* R3* D35* D48*S51}*~{D410* P46* S52* R8* S62* P56* R5*
F410}*~{D410* P46* S52* S62* P56* R5*R7* F413}*~{D410* P46* S52* R10*
S62* P56* R5* F414}*~{D410* P46* S52* S62*P56* R5* F414* D51* R7}*~{D410*
P46* S52* S62* P56* R5* D510* F414* P61* R7}*~{D410* P46* S52* D40* S50*
R10* D30* P40* R8* S62* P56* F411}*~{D410* P46*S52* D40* S50* R10* D30*
P40* R8* S62* P56* F410}*~{D410* P46* S52* D40* S50*R10* P40* S62* P56*
F47* R7* D31}*~{D410* P46* S52* D40* R10* R8* S62* P56*D51* F48}*~{D410*
P46* S52* D40* R10* R8* S62* P56* F411}*~{D410* P46* S52*D40* R10* S62*
P56* R7* F412}*~{D410* P46* S52* D40* R10* S62* P56* R7* F413}*~{D410*
P46* S52* D40* R10* S62* P56* F414* D51* R7}*~{D410* P46* S52* R10*D41*
R8* S62* P56}*~{D410* P46* S52* D40* S50* R10* P40* D33* R3* S62*
P56*F47}*~{D410* P46* S52* S41* D40* S50* R10* P40* R3* D35* S62*
P56}*~{D410*P46* S52* S41* D40* S50* P40* R3* D35* R8* S62* P56* D51*
F48}*~{D410* P46*S52* S41* D40* S50* P40* R3* D35* S62* P56* F414* D51*
R7}*~{D410* P46* S52*S41* D40* S50* P40* R3* D35* S62* P56* D510* F414*
R7* P62}*~{D410* P46* S52*D40* S50* P40* R3* R8* S62* P56* D510* F414*
P63}
V [7]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*

P36*P46* P50*~{S52}*~{D410* S52* D40* S50* S62* P56}*~{D410* S52* D40* S50* R2*S62* P56}*~{D410* S52* R10* S62* P56}*~{D410* S52* D40* R10* S62* P56}*~{D40*S50* P40* R3}*~{D410* S52* D40* S50* R2* P40* S62* P56}*~{D410* S52* S62* P56*D51}*~{D410* S52* D40* S50* R10* D30* P40* S62* P56* F414}*~{D410* S52* D40*S50* P40* R3* S62* P56* D51}*~{S41* D40* S50* P40* R3* D35}*~{D410* S52* S41*D40* S50* P40* R3* D35* S62* P56* R6* D510* F414}*~{S41* D40* S50* P40* R3*D35* D48* S51}*~{D410* S52* R8* S62* P56* R5* F410}*~{D410* S52* S62* P56* R5*R7* F413}*~{D410* S52* R10* S62* P56* R5* F414}*~{D410* S52* S62* P56* R5*F414* D51* R7}*~{D410* S52* S62* P56* R5* D510* F414* P61* R7}*~{D410* S52*D40* S50* R10* D30* P40* R8* S62* P56* F411}*~{D410* S52* D40* S50* R10* D30*P40* R8* S62* P56* F410}*~{D410* S52* D40* S50* R10* P40* S62* P56* F47* R7*D31}*~{D410* S52* D40* R10* R8* S62* P56* D51* F48}*~{D410* S52* D40* R10* R8*S62* P56* F411}*~{D410* S52* D40* R10* S62* P56* R7* F412}*~{D410* S52* D40*R10* S62* P56* R7* F413}*~{D410* S52* D40* R10* S62* P56* F414* D51* R7}*~{D410* S52* R10* D41* R8* S62* P56}*~{D410* S52* D40* S50* R10* P40* D33* R3*S62* P56* F47}*~{D410* S52* S41* D40* S50* R10* P40* R3* D35* S62* P56}*~{D410* S52* S41* D40* S50* P40* R3* D35* R8* S62* P56* D51* F48}*~{D410* S52*S41* D40* S50* P40* R3* D35* S62* P56* F414* D51* R7}*~{D410* S52* S41* D40*S50* P40* R3* D35* S62* P56* D510* F414* R7* P62}*~{D410* S52* D40* S50* P40*R3* R8* S62* P56* D510* F414* P63}

V [7]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P50*~{D40* S50}*~{P46* S52}*~{}*~{R10}*~{D410* P46* S52* D40* S50* S62* P56}*~{D410* P46* S52* D40* S50* S62* P56}*~{P46* S52* D40* S50* R2* P40}*~{D410*P46* S52* D40* S50* R2* S62* P56}*~{D410* P46* S52* R5}*~{D410* P46* S52* R10*S62* P56}*~{D410* P46* S52* D40* R10* S62* P56}*~{P46* D40* S50* P40* R3}*~{D410* P46* S52* P51* R5}*~{D410* P46* S52* D40* S50* R2* P40* S62* P56}*~{D410* P46* S52* S62* P56* D51}*~{D410* P46* S52* D40* S50* R10* D30* P40* S62*P56* F414}*~{D410* P46* S52* D40* S50* P40* R3* S62* P56* D51}*~{P46* S41*D40* S50* P40* R3* D35}*~{D410* P46* S52* S41* D40* S50* P40* R3* D35* S62*P56* R6* D510* F414}*~{P46* S41* D40* S50* P40* R3* D35* D48* S51}*~{D410*P46* S52* R8* S62* P56* R5* F410}*~{D410* P46* S52* S62* P56* R5* R7* F413}*~{D410* P46* S52* R10* S62* P56* R5* F414}*~{D410* P46* S52* S62* P56* R5*F414* D51* R7}*~{D410* P46* S52* S62* P56* R5* D510* F414* P61* R7}*~{D410*P46* S52* D40* S50* R10* D30* P40* R8* S62* P56* F411}*~{D410* P46* S52* D40*S50* R10* D30* P40* R8* S62* P56* F410}*~{D410* P46* S52* D40* S50* R10* P40*S62* P56* F47* R7* D31}*~{D410* P46* S52* D40* R10* R8* S62* P56* D51* F48}*~{D410* P46* S52* D40* R10* R8* S62* P56* F411}*~{D410* P46* S52* D40* R10*S62* P56* R7* F412}*~{D410* P46* S52* D40* R10* S62* P56* R7* F413}*~{D410*P46* S52* D40* R10* S62* P56* F414* D51* R7}*~{D410* P46* S52* R10* D41* R8*S62* P56}*~{D410* P46* S52* D40* S50* R10* P40* D33* R3* S62* P56* F47}*~{D410* P46* S52* S41* D40* S50* R10* P40* R3* D35* S62* P56}*~{D410* P46* S52*S41* D40* S50* P40* R3* D35* R8* S62* P56* D51* F48}*~{D410* P46* S52* S41*D40* S50* P40* R3* D35* S62* P56* F414* D51* R7}*~{D410* P46* S52* S41* D40*S50* P40* R3* D35* S62* P56* D510* F414* R7* P62}*~{D410* P46* S52* D40* S50*P40* R3* R8* S62* P56* D510* F414* P63}

V [7]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*~{P46* S52* P50}*~{P50}*~{D410* P46* S52* S62* P56}*~{}*~{D410* P46* S52*P50* D40* S50* S62* P56}*~{D410* P46* S52* P50* D40* S50* S62* P56}*~{D410*P46* S52* P50* D40* S50* R2* S62* P56}*~{D410* P46* S52* S62*

P56* P51* R5}*~{D410* P46* S52* P50* R10* S62* P56}*~{D410* P46* S52* P50* D40* R10* S62*P56}*~{P46* P50* D40* S50* P40* R3}*~{D410* P46* S52* P50* D40* S50* R2* P40*S62* P56}*~{D410* P46* S52* P50* S62* P56* D51}*~{D410* P46* S52* P50* D40*S50* R10* D30* P40* S62* P56* F414}*~{D410* P46* S52* R10* S62* P56* R4* P53}*~{D410* P46* S52* P50* D40* S50* P40* R3* S62* P56* D51}*~{P46* S41* P50*D40* S50* P40* R3* D35}*~{D410* P46* S52* S41* P50* D40* S50* P40* R3* D35*S62* P56* R6* D510* F414}*~{P46* S41* P50* D40* S50* P40* R3* D35* D48* S51}*~{D410* P46* S52* R8* S62* P56}*~{D410* P46* S52* P50* R8* S62* P56* R5*F410}*~{D410* P46* S52* P50* S62* P56* R5* R7* F413}*~{D410* P46* S52* P50*R10* S62* P56* R5* F414}*~{D410* P46* S52* P50* S62* P56* R5* F414* D51* R7}*~{D410* P46* S52* P50* S62* P56* R5* D510* F414* P61* R7}*~{D410* P46* S52*P50* D40* S50* R10* D30* P40* R8* S62* P56* F411}*~{D410* P46* S52* P50* D40*S50* R10* D30* P40* R8* S62* P56* F410}*~{D410* P46* S52* P50* D40* S50* R10*P40* S62* P56* F47* R7* D31}*~{D410* P46* S52* P50* D40* R10* R8* S62* P56*D51* F48}*~{D410* P46* S52* P50* D40* R10* R8* S62* P56* F411}*~{D410* P46*S52* P50* D40* R10* S62* P56* R7* F412}*~{D410* P46* S52* P50* D40* R10* S62*P56* R7* F413}*~{D410* P46* S52* P50* D40* R10* S62* P56* F414* D51* R7}*~{D410* P46* S52* P50* R10* D41* R8* S62* P56}*~{D410* P46* S52* P50* D40* S50*R10* P40* D33* R3* S62* P56* F47}*~{D410* P46* S52* S41* P50* D40* S50* R10*P40* R3* D35* S62* P56}*~{D410* P46* S52* S41* P50* D40* S50* P40* R3* D35*R8* S62* P56* D51* F48}*~{D410* P46* S52* S41* P50* D40* S50* P40* R3* D35*S62* P56* F414* D51* R7}*~{D410* P46* S52* S41* P50* D40* S50* P40* R3* D35*S62* P56* D510* F414* R7* P62}*~{D410* P46* S52* P50* D40* S50* P40* R3* R8*S62* P56* D510* F414* P63}*~{D410* P46* S52* S62* P56* R4* R6* D510* F414*P53}

V [7]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P46* S52* P50*~{}*~{D410* D40* S50* S62* P56}*~{D410* D40* S50* S62* P56}*~{D40* S50* R2* P40}*~{D410* D40* S50* R2* S62* P56}*~{D410* R10* S62* P56}*~{D410* D40* R10* S62* P56}*~{D410* D40* S50* R2* P40* S62* P56}*~{D410* S62*P56* D51}*~{D410* D40* S50* R10* D30* P40* S62* P56* F414}*~{D410* D40* S50*P40* R3* S62* P56* D51}*~{D410* S41* D40* S50* P40* R3* D35* S62* P56* R6*D510* F414}*~{D410* R8* S62* P56* R5* F410}*~{D410* S62* P56* R5* R7* F413}*~{D410* R10* S62* P56* R5* F414}*~{D410* S62* P56* R5* F414* D51* R7}*~{D410* S62* P56* R5* D510* F414* P61* R7}*~{D410* D40* S50* R10* D30* P40* R8*S62* P56* F411}*~{D410* D40* S50* R10* D30* P40* R8* S62* P56* F410}*~{D410*D40* S50* R10* P40* S62* P56* F47* R7* D31}*~{D410* D40* R10* R8* S62* P56*D51* F48}*~{D410* D40* R10* R8* S62* P56* F411}*~{D410* D40* R10* S62* P56*R7* F412}*~{D410* D40* R10* S62* P56* R7* F413}*~{D410* D40* R10* S62* P56*F414* D51* R7}*~{D410* R10* D41* R8* S62* P56}*~{D410* D40* S50* R10* P40*D33* R3* S62* P56* F47}*~{D410* S41* D40* S50* R10* P40* R3* D35* S62* P56}*~{D410* S41* D40* S50* P40* R3* D35* R8* S62* P56* D51* F48}*~{D410* S41*D40* S50* P40* R3* D35* S62* P56* F414* D51* R7}*~{D410* S41* D40* S50* P40*R3* D35* S62* P56* D510* F414* R7* P62}*~{D410* D40* S50* P40* R3* R8* S62*P56* D510* F414* P63}

V [7]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* S62* P56*~{}*~{P50* D40* S50}*~{P50* D40* S50}*~{P50* D40*S50* R2}*~{P51* R5}*~{P50* R10}*~{P50* D40* R10}*~{P50* D40* S50* R2* P40}*~{P50* D51}*~{P50* D40* S50* R10* D30* P40* F414}*~{R10* R4* P53}*~{P50* D40*S50* P40* R3* D51}*~{S41* P50* D40* S50* P40* R3* D35* R6* D510* F414}*~{R8}*~{P50* R8* R5* F410}*~{P50* R5* R7* F413}*~{P50*

R10* R5* F414}*~{P50* R5*F414* D51* R7}*~{P50* R5* D510* F414* P61*
R7}*~{P50* D40* S50* R10* D30* P40*R8* F411}*~{P50* D40* S50* R10* D30*
P40* R8* F410}*~{P50* D40* S50* R10* P40*F47* R7* D31}*~{P50* D40* R10*
R8* D51* F48}*~{P50* D40* R10* R8* F411}*~{P50* D40* R10* R7*
F412}*~{P50* D40* R10* R7* F413}*~{P50* D40* R10* F414*D51* R7}*~{P50*
R10* D41* R8}*~{P50* D40* S50* R10* P40* D33* R3* F47}*~{S41*P50* D40*
S50* R10* P40* R3* D35}*~{S41* P50* D40* S50* P40* R3* D35* R8*
D51*F48}*~{S41* P50* D40* S50* P40* R3* D35* F414* D51* R7}*~{S41* P50*
D40* S50*P40* R3* D35* D510* F414* R7* P62}*~{P50* D40* S50* P40* R3* R8*
D510* F414*P63}*~{R4* R6* D510* F414* P53}

V [7]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* S62* P56*~{D40* S50}*~{D40* S50}*~{D40* S50*
R2}*~{R10}*~{D40* R10}*~{D40* S50* R2* P40}*~{D51}*~{D40* S50* R10* D30*
P40* F414}*~{D40* S50* P40* R3* D51}*~{S41* D40* S50* P40* R3* D35* R6*
D510* F414}*~{R8*R5* F410}*~{R5* R7* F413}*~{R10* R5* F414}*~{R5* F414*
D51* R7}*~{R5* D510*F414* P61* R7}*~{D40* S50* R10* D30* P40* R8*
F411}*~{D40* S50* R10* D30* P40*R8* F410}*~{D40* S50* R10* P40* F47* R7*
D31}*~{D40* R10* R8* D51* F48}*~{D40* R10* R8* F411}*~{D40* R10* R7*
F412}*~{D40* R10* R7* F413}*~{D40* R10*F414* D51* R7}*~{R10* D41*
R8}*~{D40* S50* R10* P40* D33* R3* F47}*~{S41* D40*S50* R10* P40* R3*
D35}*~{S41* D40* S50* P40* R3* D35* R8* D51* F48}*~{S41*D40* S50* P40*
R3* D35* F414* D51* R7}*~{S41* D40* S50* P40* R3* D35* D510*F414* R7*
P62}*~{D40* S50* P40* R3* R8* D510* F414* P63}

V [7]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* S62* P56*~{}*~{R10* R4* P53}*~{R8}*~{R4* R6* D510*
F414* P53}

V [7]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* S62* P56*~{D40* S50* R2}*~{R10}*~{D40*
R10}*~{D40* S50*R2* P40}*~{D40* S50* R10* D30* P40* F414}*~{D40* S50*
P40* R3* D51}*~{S41*D40* S50* P40* R3* D35* R6* D510* F414}*~{R8* R5*
F410}*~{R5* R7* F413}*~{R10* R5* F414}*~{R5* F414* D51* R7}*~{R5* D510*
F414* P61* R7}*~{D40* S50*R10* D30* P40* R8* F411}*~{D40* S50* R10* D30*
P40* R8* F410}*~{D40* S50* R10*P40* F47* R7* D31}*~{D40* R10* R8* D51*
F48}*~{D40* R10* R8* F411}*~{D40* R10*R7* F412}*~{D40* R10* R7*
F413}*~{D40* R10* F414* D51* R7}*~{R10* D41* R8}*~{D40* S50* R10* P40*
D33* R3* F47}*~{S41* D40* S50* R10* P40* R3* D35}*~{S41* D40* S50* P40*
R3* D35* R8* D51* F48}*~{S41* D40* S50* P40* R3* D35*F414* D51*
R7}*~{S41* D40* S50* P40* R3* D35* D510* F414* R7* P62}*~{D40* S50*P40*
R3* R8* D510* F414* P63}

V [6]

D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* R10* S62* P56* F47*~{R7}*~{S60* F40* P50}*~{F414}*~{S60*
F40* P51*R5}*~{R8}*~{S60* F40* R4* P53}

V [5]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* S50* P40*~{P51* R5}*~{R10* D30* S62* P56*
F414}*~{S41* R3* D35* S62* P56* R6* D510* F414}*~{R10* P31* D30* R2* S40*
S62* P56}*~{R2* D35* R8* S62* P56* D510* F414* P63}*~{R10* P31* D30* R2*
S40* S62* P56*F47}*~{R10* P31* D30* R2* S40* S62* P56* F414}*~{R10* D30*
R8* S62* P56* F411}*~{R10* D30* R8* S62* P56* F410}*~{R10* S62* P56* F47*
R7* D31}*~{R10* D33*R3* S62* P56* F47}*~{S41* R10* R3* D35* S62*

P56}*~{S41* R3* D35* R8* S62*P56* D51* F48}*~{S41* R3* D35* S62* P56*
F414* D51* R7}*~{S41* R2* R8* S62*P56* F44}*~{S41* R2* R8* S62* P56* F47*
D51}*~{P31* D30* R2* S40* S62* P56*D510* F414* R7* P62}*~{S41* R3* D35*
S62* P56* D510* F414* R7* P62}*~{R3* R8*S62* P56* D510* F414* P63}
V [5]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* S50* P40* R3* S62* P56*~{D51}*~{S41* D35*
R6* D510*F414}*~{R10* D33* F47}*~{S41* R10* D35}*~{S41* D35* D510* F414*
R7* P62}*~{R8* D510* F414* P63}
V [5]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*P50* D40* S50* P40*~{R2}*~{P46* S52* R10* D33* R3}*~{D410* P46* S52*
P51* R5}*~{S41* R3* D35}*~{D410* P46* S52* R10* D30* S62* P56*
F414}*~{P46* S52* R10*D30* D41* R8}*~{D410* P46* S52* S41* R3* D35* S62*
P56* R6* D510* F414}*~{D410* P46* S52* R10* P31* D30* R2* S40* S62*
P56}*~{D410* P46* S52* R2* D35*R8* S62* P56* D510* F414* P63}*~{D410*
P46* S52* R10* P31* D30* R2* S40* S62*P56* F47}*~{D410* P46* S52* R10*
P31* D30* R2* S40* S62* P56* F414}*~{D410*P46* S52* R10* D30* R8* S62*
P56* F411}*~{D410* P46* S52* R10* D30* R8* S62*P56* F410}*~{D410* P46*
S52* R10* S62* P56* F47* R7* D31}*~{D410* P46* S52*R10* D33* R3* S62*
P56* F47}*~{D410* P46* S52* S41* R10* R3* D35* S62* P56}*~{D410* P46* S52*
S41* R3* D35* R8* S62* P56* D51* F48}*~{D410* P46* S52*S41* R3* D35* S62*
P56* F414* D51* R7}*~{D410* P46* S52* S41* R2* R8* S62*P56* F44}*~{D410*
P46* S52* S41* R2* R8* S62* P56* F47* D51}*~{D410* P46* S52*P31* D30* R2*
S40* S62* P56* D510* F414* R7* P62}*~{D410* P46* S52* S41* R3*D35* S62*
P56* D510* F414* R7* P62}*~{D410* P46* S52* R3* R8* S62* P56* D510*F414*
P63}
V [5]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*P46* P50* D40* S50* P40* R3*~{S52* R10}*~{D410* S52* S62* P56*
D51}*~{R2* D37*D48* S51}*~{R2* D48* S51* D38}*~{D410* S52* P51*
R5}*~{D410* S52* S41* D35*P51* R5}*~{S41* R2* D48* S51}*~{D410* S52* S41*
D35* S62* P56* R6* D510* F414}*~{S41* D35* D48* S51}*~{D410* S52* R10*
D33* S62* P56* F47}*~{D410* S52* S41*R10* D35* S62* P56}*~{D410* S52* S41*
D35* S62* P56* D510* F414* R7* P62}*~{D410* S52* R8* S62* P56* D510* F414*
P63}
V [5]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* S41* P50* D40* S50* P40* R3* D35* S62* P56*~{F414*
R7}*~{R6*D510* F414}*~{R10}*~{R8* D51* F48}
V [5]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* S50* P40* S62* P56*~{R2}*~{R10* D30*
F414}*~{R3*D51}*~{S41* R3* D35* R6* D510* F414}*~{R10* D30* R8*
F411}*~{R10* D30* R8*F410}*~{R10* F47* R7* D31}*~{R10* D33* R3*
F47}*~{S41* R10* R3* D35}*~{S41*R3* D35* D510* F414* R7* P62}*~{R3* R8*
D510* F414* P63}
V [5]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* S50* S62* P56*~{R2}*~{R10* D30* P40*
F414}*~{P42*R10* R2}*~{S41* P40* R3* D35* R6* D510* F414}*~{R10* D30*
P40* R8* F411}*~{R10* D30* P40* R8* F410}*~{R10* P40* F47* R7*
D31}*~{R10* P40* D33* R3* F47}*~{S41* R10* P40* R3* D35}*~{S41* P40* R3*
D35* R8* D51* F48}*~{S41* P40* R3*D35* F414* D51* R7}*~{S41* P40* R3*

D35* D510* F414* R7* P62}*~{P40* R3* R8*D510* F414* P63}
V [5]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* R8* S62* P56* F46*~{S60* F40* P51* R5}*~{S60* F40* P50*
D40* S50*R2* P43}*~{F40* R10}
V [5]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*P46* S52* P50* D40* S50*~{D410}*~{D410* R2}*~{R10* P31* D30* R2* S40*
P40}*~{R10* P40* D33* R3}*~{S41* R10* P40* R3* D35}*~{R10* D30* P40* D41*
R8}*~{D410* R2* P41* P52* R4}*~{D410* P42* R10* R2* S62* P56*
F47}*~{D410* P42* R10*R2* S62* P56* F414}*~{D410* P42* R2* P51*
R5}*~{D410* P42* R2* R4* P53}
V [4]
D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* S62* P56* D51*~{S60* P50}*~{R10* F414* R7}
V [3]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* S62* P56* D510* F414* R7* P62*~{F412}*~{S60* F40* P50* D40*
S50*P31* D30* R2* S40* P40}*~{S60* F40* P50* D40* S50* R2* P41}*~{S60*
F40* S41*P50* D40* S50* P40* R3* D35}*~{R10}
V [2]
D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* F42*~{D310*
S42*D410* P46* S52* R10* S62* P56* F414* R9}
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* S41* P50* D40* S50* P40* R3* D35* S62* P56* D51* R9
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* S41* P50* D40* S50* P40* R3* D35* S62* P56* F42* R9
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* S41* P50* D40* S50* P40* R3* D35* R8* S62* P56* F44
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* S41* P50* D40* S50* P40* R3* D35* R8* S62* P56* F46
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* S41* P50* D40* S50* R10* P40* R3* D35* S62* P56* F47
V [1]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* S62* P56* D510* F414* F42* R9* R7* P62
V [1]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* R8* S62* P56* D510* F414* R7* P62* F43
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* S62* P56* R5* D51* R9
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* R8* S62* P56* R5* F47* D51
V [1]
D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* R10* S62* P56* F47* D51* R9
V [1]

D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* R10* R8* S62* P56* F47* F43
V [1]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* R10* R8* S62* P56* F47* F44
V [1]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* R10* R8* S62* P56* F47* D51* F48
V [1]
D310* F40* S42* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* S62* P56* D510* F414* D51* R9* R7* P62
V [1]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* R10* R8* S62* P56* F47* F46

CONCEPT FOR CLASS Yb_3S_4 :

[3]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
R8*~{D410* P46* S52* S62* P56}*~{D410* P46* S52* S62* P56* F411}*~{S60*
F40* P46*S52* P50* D40* R10}*~{S60* F40* D410* P46* S52* P50* D41*
R5}*~{S60* F40*D410* P46* S52* P50* D40* S50* R10* D30* P40* S62* P56} V
[2]S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60*
B3* P36*P46* S52* P50* D40* S50* R10* P40*~{R3}*~{P31* D30* R2*
S40}*~{D410* D30* S62*P56* F414}*~{D410* D30* R8* S62* P56* F410}*~{D410*
S62* P56* F47* R7* D31}*~{D410* D30* P51* R5}
V [2]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* R10* S62* P56* F414*~{R8}*~{S60* F40* P50* D40* S50* D30*
P40}*~{F40* D51* R7}*~{F47}*~{S60* F40* P50* R5}*~{S60* F40* P50* D40*
S50* P31* D30*R2* S40* P40}*~{S60* F40* P51* R5}*~{S60* F40* P50* D40*
D51* R7}*~{S60* F40*P42* P50* D40* S50* R2}*~{D510* R7* P62}*~{F42* R9}
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*P46* S52* P50* D40* S50* R10* D30* P40* D41* R8
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* S50* R10* D30* P40* R8* S62* P56* F411
V [1]
D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* R10* R8* S62* P56*~{S60* P50* D40* D51* F48}*~{S60*
P50* D40*F411}*~{S60* P50* D41}* ~{F410}* ~{F46}*~ {D510* F414* P63}
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* R8* S62* P56*~{D510* F414* P63}*~{P50* R5*
F410}*~{P50* R5*F47* D51}*~{P51* R5* F46}*~{S41* P50* D40* S50* P40* R3*
D35* F44}*~{S41* P50*D40* S50* P40* R3* D35* F46}*~{P50* D40* S50* R10*
D30* P40* F410}*~{P50* D40*R10* D51* F48}*~{P50* D40* R10* F411}*~{P50*
R10* D41}*~{S41* P50* D40* S50*P40* R3* D35* D51* F48}*~{P52* R4*
F44}*~{S41* P50* D40* S50* R2* P40* F44}*~{S41* P50* D40* S50* R2* P40*
F47* D51}*~{P50* D40* S50* R2* P43* F46} V [1]D310* S42* D50* S12* S22*
P26* S32* F50* D60* S70* B2* P60* B3* P36* D410*P46* S52* R10* R8* S62*
P56* F414* F411

CONCEPT FOR CLASS Yb_3Se_4 :

[4]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* D410*P46* S52* S62* P56*~{F40}*~{}
V [3]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* R10* S62* P56*~{S50* P40}*~{S50* R2* P41}*~{P42*S50* R2}*~{R8* D51* F48}*~{R8* F411}*~{R7* F412}*~{R7* F413}*~{F414* D51* R7}
V [3]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* R10* S62* P56*~{S50* P40}*~{S50* R2* P41}*~{P42*S50* R2}*~{S50* P40* F47* R7* D31}*~{R8* D51* F48}*~{R8* F411}*~{R7* F412}*~{R7* F413}*~{F414* D51* R7}
V [3]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* R10* S62* P56*~{D40* S50* P40}*~{D40* S50* R2* P41}*~{P42* D40* S50* R2}*~{R5* F414}*~{D40* R8* D51* F48}*~{D40* R8* F411}*~{D40*R7* F412}*~{D40* R7* F413}*~{D40* F414* D51* R7}*~{D41* R8}
V [3]D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* D410*P46* S52* R10* S62* P56* F414*~{}*~{F40* D51* R7}*~{F47}*~{S60* F40* P50* D40*S50* P31* D30* R2* S40* P40}*~{S60* F40* P50* D40* D51* R7}*~{S60* F40* P42*P50* D40* S50* R2}*~{D510* R7* P62}*~{F40* R8* D510* P63}
V [2]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* R10* D30* P40* S62* P56* F414*~{P31* R2* S40}
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* R10* D30* P40* R8* S62* P56* F410
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P46* S52* P50* D40* R10* R8*~{D41}*~{D410* S62* P56* D51* F48}*~{D410* S62*P56* F411}
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* R10* D30* P40* R8* S62* P56*~{F411}
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* R10* R8* S62* P56*~{D51* F48}*~{F411}
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* R10* D30* P40* S62* P56* F414* D51* R7

CONCEPT FOR CLASS $CaFe_2O_4$:

[10]
D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* R10* S62* P56*~{S60* P50* D40* S50* R2* P41}*~{S60* P50* D40*S50* D30* P40* F414}*~{S60* R4* P53}*~{S60* P50* D40* S50* P31* D30* R2* S40*P40}*~{S60* P50* R5* F414}*~{S60* P50* D40* S50* P31* D30* R2* S40* P40* F47}*~{S60* P50* D40* S50* P31* D30* R2* S40* P40* F414}*~{S60* P51* R5* F47}*~{S60* P51* R5* F414}*~{S60* S41* P50* D40*

S50* P40* R3* D35* F47}*~{S60* P50*D40* S50* D30* P40* R8* F411}*~{S60* P50* D40* S50* D30* P40* R8* F410}*~{S60* P50* D40* S50* P40* D33* R3* F47}*~{S60* S41* P50* D40* S50* P40* R3*D35}*~{S60* P42* P50* D40* S50* R2* F47}*~{S60* P42* P50* D40* S50* R2* F414}*~{F47* D51* R9}*~{R8* D510* F414* P63}*~{S60* P50* D40* S50* D30* P40* F414*D51* R7}

V [10]

D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* S62* P56*~{S60}*~{S60* P50}*~{R8* D510* F414* P63}*~{S60* P50*D40* S50* R10* D30* P40* R8* F410}*~{R10* F47* D51* R9}*~{S60* P50* D40* S50*R10* D30* P40* F414* D51* R7}

V [6]

D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* D410*P46* S52* R8* S62* P56*~{}*~{S60* F40* P50* R5* F410}*~{S60* F40* P50* D40*S50* R10* D30* P40* F411}*~{S60* F40* P50* D40* S50* R10* D30* P40* F410}*~{S60* F40* P50* D40* R10}*~{R10* F414* F411}

V [5]

D310* S42* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* D410* P46*S52* S62* P56* D51*~{D50* R8* F47}*~{S60* F40* D50* P50* D40* S50* P40* R3}*~{S60* F40* D50* P50* R5* R9}*~{S60* F40* D50* P50* R5* F414* R7}*~{F40* D50*R10* F47* R9}*~{F40* D510* F414* R9* R7* P62}*~{S60* F40* D50* P50* D40* S50*R10* D30* P40* F414* R7}*~{D50* R10* R8* F414* F48}

V [4]

D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* D410*P46* S52* R10* S62* P56* F47* R7

V [2]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* S62* P56* D51*~{R8* R5* F47}*~{R5* R9}*~{R5* F414* R7}*~{S41* D40* S50* P40* R3* D35* R9}*~{S41* D40* S50* P40* R3* D35* F414* R7}*~{S41* D40* S50* R2* P40* R8* F47}*~{F48}*~{D40* S50* R10* D30* P40* F414*R7}

V [2]

D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* D410*P46* S52* R8* S62* P56* F411*~{S60* F40* P50* D40* S50* R10* D30* P40}*~{R10*F414}

V [2]

D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* R10* S62* P56* F414* D51* R7*~{S60* P50* D40* S50* D30* P40}

V [2]

D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* D410*P46* S52* R10* S62* P56* F414* F47*~{R8* D51}

V [1]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* R10* P40* S62* P56* F47* R7* D31

V [1]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P46* S52* P50* D40* R10* D41* R8*~{S50* D30* P40}

V [1]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* R10* R8* S62* P56* D51* F48

V [1]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* R10* R8* S62* P56* F411*~{S50* D30* P40}

V [1]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* R10* S62* P56* R7* F412
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* R10* S62* P56* R7* F413
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* R10* S62* P56* F414* D51* R7*~{S50* D30*
P40}
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* R10* D41* R8* S62* P56
V [1]
D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* R10* R8* S62* P56* F46

V [1]
D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* R10* R8* S62* P56* F410*~{S60* P50* D40* S50* D30*
P40}
V [1]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* R10* R8* S62* P56* F47* F411
V [1]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* R10* R8* S62* P56* F47*~{F43}*~{F44}*~{D51*
F48}*~{F46}*~{F414* D51}
V [1]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* R10* R8* S62* P56* F47*~{F43}*~{F44}*~{D51*
F48}*~{F46}*~{F414* D51}
V [1]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* R10* S62* P56* F47* R7* F412
V [1]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* R10* S62* P56* F47* R7* F413
V [1]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* S62* P56* D510* F414* R7* F412* P62
V [1]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* R10* S62* P56* D510* F414* R7* P62

CONCEPT FOR CLASS another_structure :

[22]
S60* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*~{P50* D40* S50* P40}*~{D310}*~{P50* D40* S50* R2* P40* D35}
V [18]
P50* D40* S50*~{S60* F40* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60*
B3*P40}*~{S60* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60*
B3*P36* P40}*~{S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60*
S70* B2*P60* B3* P36}*~{S60* D310* F40* S42* D50* S12* S22* P26* S32* F50*
D60* S70*B2* P60* B3* P36* D410* P46* S52* S62* P56}*~{S60* D310* F40*

S42* D50* S12*S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* P46* S52* R2* P40}*~{S60* F40*D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* S41* P40* R3* D35}*~{S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*P36* P46* S52* R10* P31* D30* R2* S40* P40}*~{S60* D310* F40* S42* D50* S12*S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* P40* R3* D35}*~{S60* F40* S42*D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* R2* P40* D35}*~{S60* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* S41*P40* R3* D35}*~{S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70*B2* P60* B3* P36* S41* R2* P40}*~{S60* D310* F40* S42* D50* S12* S22* P26*S32* F50* D60* S70* B2* P60* B3* P36* D410* P46* S52* R2* P40* P51* R5}*~{S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P31* D30* R2* S40* P40* R3}*~{S60* D310* F40* S42* D50* S12* S22* P26* S32*F50* D60* S70* B2* P60* B3* P36* R2* P40* D36* P41}*~{S60* D310* F40* S42*D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* R2* P40* R3* D35}*~{S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*P36* R10* D30* R2* P40* P41}*~{S60* D310* F40* S42* D50* S12* S22* P26* S32*F50* D60* S70* B2* P60* B3* P36* P46* R2* P40* R3* D37* D48* S51}*~{S60* D310*F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* P46* R2*P40* R3* D48* S51* D38}*~{S60* D310* F40* S42* D50* S12* S22* P26* S32* F50*D60* S70* B2* P60* B3* P36* P46* S41* R2* P40* R3* D48* S51}*~{S60* D310* F40*D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* S41* R2* P40* R3*D35}*~{S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60*B3* P36* S41* R2* P40* D35}*~{S60* D310* F40* S42* D50* S12* S22* P26* S32*F50* D60* S70* B2* P60* B3* P36* D410* P46· S52* R10* P31* D30* R2* S40* P40*S62* P56* F47}*~{S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70*B2* P60* B3* P36* D410* P46* S52* R10* P31* D30* R2* S40* P40* S62* P56* F414}*~{S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*P36* D410* P46* S52* P31* D30* R2* S40* P40* S62* P56* D510* F414* R7* P62}

V [16]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P50* D40* S50*~{R2}*~{P40}*~{P46* S52* P40}*~{R2* P40}*~{P40* R3}*~{R2* P40*D36* P41}*~{R10* D30* R2* P40* P41}

V [14]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P46* S52* P50*~{D410* S62* P56}*~{D40* S50}*~{D40* S50* P40}*~{D410* R10* S62*P56}*~{D410* D40* R10* S62* P56}*~{D40* S50* R10* P40}*~{D410* P51* R5}*~{D40* R10* R8}*~{D410* D41* R8* R5}

V [14]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P50* D40* S50* P40*~{}*~{P46* S52}

V [8]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P50* R10*~{P46* S52* D40* S50* P31* D30* R2* S40* P40}*~{D410* P46* S52* S62*P56}*~{D410* P46* S52* D40* S62* P56}*~{P46* S52* D40* S50* P40}*~{D410* P46*S52* D40* S50* R2* P41* S62* P56}*~{D410* P46* S52* D40* S50* D30* P40* S62*P56* F414}*~{D40* S50* D30* R2* P40* P41}*~{P46* S52* D40* S50* D30* P40* D41*R8}*~{P46* S52* D40* R8}*~{D410* P46* S52* D40* S50* P31* D30* R2* S40* P40*S62* P56* F47}*~{D410* P46* S52* D40* S50* P31* D30* R2* S40* P40* S62* P56*F414}*~{D410* P46* S52* S41* D40* S50* P40* R3* D35* S62* P56* F47}*~{D410*P46* S52* D40* S50* D30* P40* R8* S62* P56* F411}*~{D410* P46* S52* D40* S50*D30* P40* R8* S62* P56* F410}*~{D410* P46* S52* D40* S50* P40* S62* P56* F47*R7* D31}*~{D410* P46*

S52* D40* S50* R2* P41* S62* P56* F47}*~{D410* P46* S52*D40* S50* D30* P40* R8* S62* P56}
V [7]
S60* F40* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* P50* D40*S50* R10* P40*~{D310* S42* P46* S52* P31* D30* R2* S40}*~{D310* S42* P46* S52}*~{D310* S42* D30* R2* P41}*~{D310* S42* D410* P46* S52* P31* D30* R2* S40*S62* P56* F47}*~{D310* S42* D410* P46* S52* P31* D30* R2* S40* S62* P56* F414}
V [6]
S60* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* P50*D40* S50* R2* P40*~{D36}*~{D310* P46* S52* R10* P31* D30* S40}*~{D310* S41}*~{D310* D410* P46* S52* P51* R5}*~{D310* P31* D30* S40* R3}*~{D310* D36* P41}*~{D310* R3* D35}*~{D310* R10* D30* P41}*~{D310* P46* R3* D37* D48* S51}*~{D310* P46* R3* D48* S51* D38}*~{D35* R7* D31}*~{D35* R5* D32}*~{D38* R5* D32}*~{D33* R3* D35}*~{D33* R3* D38}*~{S41* R3* D35* D38}*~{D310* S41* D35}*~{D310* D410* P46* S52* R10* P31* D30* S40* S62* P56* F47}*~{D310* D410* P46*S52* R10* P31* D30* S40* S62* P56* F414}*~{D310* D410* P46* S52* P31* D30*S40* S62* P56* D510* F414* R7* P62}
V [5]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* R4*~{P52}*~{P53}
V [5]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P50* D40* S50* R2* P40*~{P46* S52* R10* P31* D30* S40}*~{S41}*~{D410* P46*S52* P51* R5}*~{P31* D30* S40* R3}*~{D36* P41}*~{R3* D35}*~{R10* D30* P41}*~{P46* R3* D37* D48* S51}*~{P46* R3* D48* S51* D38}*~{S41* D35}*~{D410* P46*S52* P31* D30* S40* S62* P56* D510* F414* R7* P62}
V [4]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* R2*~{P43}*~{R10* P41* S62* P56}*~{P40* P51* R5}*~{P41* S62* P56* R6* D510* F414}*~{P41* R5}*~{P41* P52* R4}*~{R10* P31* D30*S40* P40* S62* P56* F47}*~{R10* P31* D30* S40* P40* S62* P56* F414}*~{S41*P40* R8* S62* P56* F44}*~{S41* P40* R8* S62* P56* F47* D51}*~{P31* D30* S40*P40* S62* P56* D510* F414* R7* P62}*~{P41* S62* P56* D510* F414* R7* P62}*~{P42* P51* R5}*~{P42* R4* P53}
V [4]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* R2* S62* P56*~{R10* P41}*~{S41* P40}*~{P43}*~{P41* R6* D510* F414}*~{R10* P31* D30* S40* P40* F47}*~{R10* P31* D30* S40*P40* F414}*~{P31* D30* S40* P40* D510* F414* R7* P62}*~{P41* D510* F414* R7*P62}
V [4]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P46* S52* P50* D40* S50* R10* P40* R3*~{D410* S41* D35* S62* P56* F47}
V [3]
D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* D30* S40*~{S60*D310* F40* S42* P46* S52* P50* D40* S50* P40}*~{S60* D310* F40* S42* P46* S52*P50* D40* S50* R10* P31* R2* P40}*~{S60* D310* F40* S42* P50* D40* S50* P31*R2* P40* R3}*~{S60* D310* F40* S42* D410* P46* S52* P50* D40* S50* R10* P31*R2* P40* S62* P56* F47}*~{S60* D310* F40* S42* D410* P46* S52* P50* D40* S50*R10* P31* R2* P40* S62* P56* F414}
V [3]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*

P36*D410* P46* S52* P50* D40* S50* R10* P40* S62* P56*~{D30* F414}*~{P31* D30* R2*S40* F47}*~{P31* D30* R2* S40* F414}*~{S41* R3* D35* F47}*~{D30* R8* F411}*~{D30* R8* F410}*~{F47* R7* D31}

V [3]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* S62* P56* D510* F414*~{P50* D40* S50* R2* P41* R6}*~{P51* R5*R6}*~{S41* P50* D40* S50* P40* R3* D35* R6}*~{P50* D40* S50* P31* D30* R2*S40* P40* R7* P62}*~{P50* D40* S50* R2* P41* R7* P62}*~{P50* D40* S50* P40*R3* R8* P63}*~{R4* R6* P53}*~{P50* D40* S50* R2* P43* R6}*~{R8* P52* R4* P63}

V [3]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* R5*~{P51}*~{S62* P56}*~{R8}*~{D40* S50* R2* P41}*~{D40*S50* R2* P43}

V [2]

S60* F40* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P50* D40* S50*P40* R4* P30

V [2]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* P40* P51* R5*~{S41}*~{R2}*~{R3}

V [2]

S60* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* P50*D40* S50* P40* R5*~{D32}*~{D310* D410* P46* S52* S41* P51}*~{D310* D410* P46*S52* R2* P51}*~{D310* D410* P46* S52* R3* P51}

V [2]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* P40* P51* R5*~{S41}*~{R2}*~{R3}

V [2]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* R2* P40* S62* P56*~{S41}*~{R10* P31* D30* S40*F47}*~{R10* P31* D30* S40* F414}*~{P31* D30* S40* D510* F414* R7* P62}

V [2]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P46* S52* P50* D40* S50* R10* P40* D33* R3

V [2]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* R10* S62* P56* F47*~{D40* S50* P31* D30* R2* S40* P40}*~{S41* D40* S50* P40* R3* D35}*~{D40* S50* P40* R7* D31}*~{D40* S50* R2* P41}

V [2]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P46* S52* S41* P50* D40* S50* R10* P40* R3* D35*~{D410* S62* P56* F47}

V [2]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* P40* R3* S62* P56* D51*~{S41* D35* R9}

V [2]

S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* S41* P50* D40* S50* P40* R3* D35* S62* P56* F414* R7

V [2]

D310* S42* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* D410* P46*S52* R8* S62* P56* D510* F414* P63*~{S60* F40* D50* P50* D40* S50* P40* R3}*~{S60* F40* D50* P52* R4}*~{R6}

V [2]

D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* R8* S62* P56* D510* F414* P63*~{S60}
V [2]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P42* P50* D40* S50* R10* R2* S62* P56
V [2]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* R10* S62* P56* R4* P53
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* S50* D30* S40* P40* P51* R5* R4* P30
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* S50* R10* P31* D30* R2* S40* P40* S62*
P56*~{F47}*~{F414}
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* S50* R10* D30* P40* P51* R5
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* S50* R10* P40* D33* R3* S62* P56* F47
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* S41* P50* D40* S50* R10* P40* R3* D35* S62* P56*~{F47}
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* S41* P50* D40* S50* P40* R3* D35* R8* S62* P56* D51*
F48
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* S62* P56* D51* F48*~{D40* R10* R8}
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* S41* P50* D40* S50* P40* R3* D35* S62* P56* F414* D51*
R7
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* S41* P50* D40* S50* P40* R3* D35* S62* P56* D510*
F414* R7*P62
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*P50* D40* S50* R2* P40* P41* D35
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*P50* D40* S50* R2* P40* D35* P43
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* S50* R2* P40* D35* R8* S62* P56* D510*
F414* P63
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P42* P50* D40* S50* R10* R2* S62* P56* F47
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*

P36*D410* P46* S52* P42* P50* D40* S50* R10* R2* S62* P56* F414
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* S62* P56* R5* D510* F414* P61* R7
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* R8* S62* P56* P52* R4* F44
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* R10* S62* P56* R4* F47* P53
V [1]
D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* R10* R8* S62* P56* D510* F414* P63
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*S41* P50* D40* S50* R2* P40* P41
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P52* R4* P53

CONCEPT FOR CLASS without_compound_AB_2Se_4 :

[12]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* S50*~{P40}*~{R10* R2* P41* S62* P56}*~{R2*
P41* S62*P56* R6* D510* F414}*~{R2* P41* R5}*~{P42* R10* R2* S62* P56*
F47}*~{P42* R10*R2* S62* P56* F414}*~{R2* P41* S62* P56* D510* F414* R7*
P62}
V [11]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*P50* D40* S50* R2*~{P40}*~{D410* P46* S52}*~{D410* P46* S52* S62*
P56}*~{P46*S52* R10* P31* D30* S40* P40}*~{P41}*~{D410* P46* S52* P42*
R10* S62* P56}*~{D410* P46* S52* P42* R10* S62* P56* F47}*~{D410* P46*
S52* P42* R10* S62*P56* F414}
V [7]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* S62* P56*~{}*~{P50* D40* S50* R2* P41* R6* D510*
F414}*~{P51*R5* R6* D510* F414}*~{S41* P50* D40* S50* P40* R3* D35* R6*
D510* F414}
V [5]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* S50* S62* P56*~{}*~{S41* P40* R3*
D35}*~{R10* P40*D33* R3* F47}*~{S41* R10* P40* R3* D35}
V [5]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* S50* S62* P56*~{}*~{S41* P40* R3*
D35}*~{R2* P41}*~{R10* P40* D33* R3* F47}*~{S41* R10* P40* R3* D35}
V [4]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P52* R4*~{R8* S62* P56* F44}*~{P53}
V [4]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*P46* S52* P50* D40* S50* R2* P40*~{R10* P31* D30* S40}*~{D410* S62*
P56}*~{D410* P31* D30* S40* S62* P56* D510* F414* R7* P62}

V [4]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* P51* R5*~{D40* S50* P40}
V [3]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*S41* P50* D40* S50* R2* P40*~{P46* R3* D48* S51}*~{P41}*~{D35}
V [3]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* R2* P43
V [3]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* D410*P46* S52* R10* R8* S62* P56* F414*~{F40* D510* P63}*~{F411}
V [3]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P42* P50* D40* S50*~{D410* P46* S52* R10* R2* S62* P56* F47}*~{D410* P46* S52*R10* R2* S62* P56* F414}
V [2]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* S41* P50* D40* S50* R2* P40* S62* P56
V [2]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* D410*P46* S52* R8* S62* P56* F47* D51*~{S60* F40* P50* R5}*~{R10* F48}
V [2]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* R2* P43* S62* P56
V [2]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* R4* P53*~{R10* S62* P56}*~{P52}
V [2]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* S62* P56* R6* D510* F414*~{P50* D40* S50* R2* P41}*~{P51* R5}*~{S41* P50* D40* S50* P40* R3* D35}
V [2]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* R8* S62* P56* D510* F414* P63*~{P50* D40* S50* R2* P40* D35}
V [2]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* S41* P50* D40* S50* P40* P51* R5
V [2]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* P50* D40* S50* R2* P40* P51* R5
V [2]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*P46* P50* D40* S50* P40* R3*~{}*~{D410* S52* S41* D35* S62* P56}*~{R2* D37*D48* S51}*~{R2* D48* S51* D38}*~{S41* R2* D48* S51}*~{D410* S52* R10* D33*S62* P56* F47}*~{D410* S52* S41* R10* D35* S62* P56}
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* S41* P50* D40* S50* R2* P40* R8* S62* P56* F44
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*D410* P46* S52* S41* P50* D40* S50* R2* P40* R8* S62* P56* F47* D51

V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* S50* R2* R8* P43* S62* P56* F46
V [1]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* R10* S62* P56* F414* F42* R9
V [1]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* R10* R8* S62* P56* F414* F47* D51
V [1]
D310* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36*
D410*P46* S52* R10* R8* S62* P56* F414* D51* F48
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* S50* R2* P41* P52* R4
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P42* P50* D40* S50* R2* R4* P53
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* S50* R2* P43* R5
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* S50* R2* P43* S62* P56* R6* D510* F414
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* R8* S62* P56* P52* R4* D510* F414* P63
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* S62* P56* R4* R6* D510* F414* P53
V [1]
D310* S42* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3* P36* D410*
P46*S52* R8* S62* P56* R6* D510* F414* P63
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* S41* P50* D40* S50* P40* R3* D35* P51* R5
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P50* D40* S50* P40* R3* R8* S62* P56* D510* F414* P63
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*D410* P46* S52* P42* P50* D40* S50* R2* P51* R5
V [1]
S60* D310* F40* S42* D50* S12* S22* P26* S32* F50* D60* S70* B2* P60* B3*
P36*P42* P50* D40* S50* R2* P41x

Feature set II. The predicting Crystal Type for Composition $A(II)B(III)_2Se_4$

CONCEPT FOR CLASS chalcopyrite :

[9]
Se11* P* S* E2*~{E1* N3* Se23}*~{N4* Se12}*~{H9* Ne1* I38* R17* N2* NM11* I12*I21}*~{Se23* I33* Ne6* I27* NM12}*~{Se23* E3* N5* H6* Ne7* NM8}*~{N4* N2* Ne5*H8* I36* R10* I39* NM9* I19* I24* I16* NM10* I25* R12}

V [5]
Se11* P* S* E2* E1* N3* Se23* N2* H8* I39* Ne4

V [4]
N2* Ne5* I39* NM9*~{H8* I19* I25* R12}*~{S* E2* H8* I19* I25* R12* Ne2}

V [3]
Se11* P* N2* H8* I39* Ne4* R7* I110* I26* NM6*~{S* E2* Se23* I33* Ne6* I27*NM12* E3* N5* I16* R14}*~{S* E2* N4* Se12* Ne5* I36* R10* I24* I16* NM10* H7}*~{S* E2* N4* Se12* Ne7* NM8* I25* H5* I37* R5* I18}

V [3]
Ne5* NM9* I19* I25* R12*~{N2* H8* I39}*~{S* E2* N2* H8* I39* Ne2}*~{Se11* S* E2*N3* Se23* N2* H8* I39* Ne2* R14* I13* F* I22}*~{Se11* S* E2* E1* N3* Se23* N2*NM8* H8* I39* Ne2* R14* I22* D* I14* I31}*~{Se11* S* E2* N3* Se23* N2* NM11*I33* H8* I39* Ne2* F* I22* I14* E13* R13}*~{Se11* S* E2* N3* Se23* N2* NM11*H8* I39* Ne2* F* I14* R13* E12* I23* I32}*~{Se11* S* E2* E1* N3* Se23* N2*NM11* H8* I39* I24* Ne2* I13* D* R13* I32}*~{Se11* S* E2* N3* Se23* R17* N2*NM12* H8* I39* Ne2* I13* F* I22* E0* I34}*~{Se11* S* E2* N3* Se23* N2* NM11*H8* I39* Ne2* R14* F* I23* I32* E11* I15}*~{Se11* S* E2* N3* Se23* N2* NM11*H8* I39* Ne2* R14* F* I23* I32* I15* E10}*~{Se11* S* E2* N3* Se23* N2* NM11*H8* I39* Ne2* R14* I13* F* I22* I32* E7}

V [3]
Se11* P* S* E2* E1* N3* Se23* N2* Ne5* H8* I39* NM9* Ne4

V [3]
Se11* P* S* E2* E1* N3* Se23* I12* I27* Ne5* H8* NM9* I34* R11*~{N2* I310}

V [3]
Se11* P* S* E2* E1* N3* Se23* NM8* I36* Ne4* R5* I13* H10* I28*~{Ne1* R17* N2}

V [2]
Se11* P* E1* N3* Se23* NM8* H8* I36* Ne4* R5* I13* I28*~{NM12* Ne5* H7* R13*I35}*~{E3* N5* H6* Ne7* I110* I26* I34* R2}*~{S* E2* Ne1* R17* N2* I22* I310*H10* NM2}*~{I24* I16* NM6* I37* D* H10* E5* N7* R6}

V [1]
Se11* P* S* E2* E1* N3* Se23* N2* I27* H6* H8* I39* Ne4* R7* I110* I26* NM6*I13* I34* R4* NM4

V [1]
Se11* P* S* E2* E1* N3* Se23* N2* I27* H6* Ne5* H8* I39* NM9* I19* I25* R12*Ne4* I13* I34* R4* NM4

V [1]
Se11* P* N3* Se23* I27* H6* Ne5* H8* NM9* I34*~{E2* E1* N4* I12* I36* R10* I24*I16* NM10* R11}*~{E2* E1* N4* I12* Ne7* NM8* I25* I37* R5* I18* R11}*~{E1* I12*I26* NM6* I37* D* E7* R11* N8* I17* R3}

V [1]
Se11* P* S* E2* E1* N3* Se23* N2* NM8* H8* I36* I39* Ne4* R7* I110* I26* NM6*R5* I13* H10* I28

V [1]
Se11* P* S* E2* E1* N3* Se23* N2* I12* I27* Ne5* H8* I39* NM9* Ne4* R7* I110*I26* NM6* I34* R11
V [1]
Se11* P* S* E2* E1* N3* Se23* N2* NM8* Ne5* H8* I36* I39* NM9* I19* I25* R12*Ne4* R5* I13* H10* I28
V [1]
Se11* P* S* E2* E1* N3* Se23* Ne6* I27* NM12* NM8* I36* Ne4* I110* H5* I37* R5*I13* R13* H10* I28* N9
V [1]
Se11* P* S* E2* E1* N3* Se23* N2* I12* I27* Ne5* H8* I39* NM9* I19* I25* R12*I34* R11
V [1]
Se11* P* S* E2* E1* N3* Se23* I12* Ne6* I27* NM12* Ne5* H8* NM9* I110* H5* I37*R13* I34* R11* N9
V [1]
Se11* P* S* E2* N4* Se12* Ne6* I27* NM12* Ne7* NM8* I25* I110* H5* I37* R5* I18*R13* N9

CONCEPT FOR CLASS spinel :

[9]
Se11* N3* Se23*~{F}*~{Ne2}*~{P* E1}*~{H8}*~{I17}*~{R17* I34}*~{P* E1* NM8* I36*Ne4* R5* I13* I28}*~{H1}*~{P* S* E2* E1* H9* Ne1* I38* R17* N2* NM11* I12* I21*I27* H6* Ne4* I13* I34* R4* NM4}
V [7]
Se11* S* E2* N3* Se23* Ne2*~{H9* Ne1* R17* N2}*~{Ne1* R17* N2* H8* I13* I22*I310* NM2}*~{H9* N2* I24* I310* I17* R9* NM3}*~{N2* NM11* Ne5* H8* I39* NM9*I19* I25* R12* R14* I13* F* I22* I32* E7}*~{E1* N2* NM11* I12* I21* Ne5* H8*I39* NM9* I19* I25* R12* D* I31* H10* R16}

Feature set II. Predicting Crystal Type for Composition $A(IV)B(II)_2Se_4$

CONCEPT FOR CLASS chalcopyrite :

[1]
I110* Ne6* I27* N9* R13* NM12* Ne7* R5* NM8* H5* S* I37* I18* I25* Se12* Se11*E2* N4* P

CONCEPT FOR CLASS olivine :

[3]
Se12* Se11* E2* N4* P*~{Ne5* H7}*~{S}*~{I37* I18* I25}*~{I37* I18* I25* Ne5* D}
V [3]
Se12* Se11* Ne5*~{E2* N4* P* H7}*~{I37}*~{S* E2* N4* P* I39* H8* N2}*~{H5* I18*I25* D* I35* R4* NM5* E6* N8}
V [1]
S* Se12* Se11* E2* N4* P* Ne5* H7* N2* Ne2* I17* R9* NM3* H9* I310* I36* R10*NM10* I16* I24
V [1]
S* I37* I18* I25* Se12* Se11* E2* N4* P* Ne5* H8* N2* I310* Ne1* R17* I13* I22*H4* R2* NM2
V [1]

I37* I18* I25* Se12* Se11* E2* N4* P* Ne5* D* H8* I16* I24* H4* R2* NM2* R6*E5* N7* NM6* Ne4

CONCEPT FOR CLASS $NiCr_2S_4$:

[4]
I18* I25*~{I37}*~{H5* I37* Se12* Se11* E2* N4* P}*~{H5* I37* Se12* Se11* E2*N4* P* Ne5* D* I35* R4* NM5* E6* N8* R2* NM2* H3}
V [4]
Se11*~{E2* N4}*~{H5* I37* I18* I25* Se12* E2* N4* P}*~{Se12* Ne5}*~{S* I37*I18* I25* Se12* E2* N4* P* Ne5* N2}*~{I37* I18* I25* Se12* E2* N4* P* Ne5* D*H8* I16* I24* H4* R2* NM2* R6* E5* N7* NM6* Ne4}*~{H5* I37* I18* I25* Se12* E2*N4* P* Ne5* D* I35* R4* NM5* E6* N8* R2* NM2* H3}
V [4]
Ne5* D* N8*~{H5* I37* I18* I25* Se12* Se11* E2* N4* P* I35* R4* NM5* E6* R2*NM2* H3}*~{I27* I37* Se12* Se11* P* H7* I17* NM6* E7* H6* I26* R3* NM9* I12*I34* R11* E1* N3}
V [2]
I37* I18* I25* Se12* Se11* E2* N4* P* Ne5* D*~{H8* I16* I24* H4* R2* NM2* R6*E5* N7* NM6* Ne4}*~{H5* I35* R4* NM5* E6* N8* R2* NM2* H3}
V [2]
I37* I18* I25* Se12* Se11* E2* N4* P*~{H5}*~{S* Ne5* N2}*~{Ne5* D* H8* I16* I24*H4* R2* NM2* R6* E5* N7* NM6* Ne4}
V [2]
I37* Se12* Se11* Ne5*~{H5}*~{S* I18* I25* E2* N4* P* H8* N2* I310* Ne1* R17*I13* I22* H4* R2* NM2}*~{I18* I25* E2* N4* P* D* H8* I16· ı24* H4* R2* NM2*R6* E5* N7* NM6* Ne4}*~{I27* P* H7* D* N8* I17* NM6* E7* H6* I26* R3* NM9* I12*I34* R11* E1* N3}*~{S* I18* I25* E2* N4* P* N2* H9* Ne1* R17* H4* R2* NM2* I12*I38* I21* NM11}*~{I27* Ne7* R5* NM8* H5* I18* I25* E2* N4* P* H7* NM9* I12*I34* R11* E1* N3}
V [1]
H5* I18* I25* Se12* Se11* Ne5* D* I35* R4* NM5* E6* N8*~{I37* E2* N4* P* R2*NM2* H3}
V [1]
H5* I37* I18* I25* Se12* Se11* E2* N4* P* Ne5* D* N8* I17* R2* NM2* H3* I26*R3* I38* NM4* E8
V [1]
H5* I18* I25* Se11* E2* N4* Ne5* D* I35* R4* NM5* E6* N8* NM6* Ne4* I34* I15*I23* R12* H10

CONCEPT FOR CLASS another_structure :

[7]
Se11* E2* N4*~{Se12* P}*~{H5* I18* I25* Ne5* D* I35* R4* NM5* E6* N8* NM6* Ne4*I34* I15* I23* R12* H10}
V [6]
I37* I18* I25*~{Se12* Se11* E2* N4* P}*~{Se12* Se11* E2* N4* P* Ne5* D}*~{I110* Ne6* I27* N9* R13* NM12* Ne7* R5* NM8* H5* S* Se12* Se11* E2* N4* P}*~{S*Se12* Se11* E2* N4* P* Ne5* H8* N2* I310* Ne1* R17* I13* I22* H4* R2* NM2}
V [5]
H5* I37* I18* I25* Se12* Se11* E2* N4* P*~{Ne7* R5* NM8}*~{Ne5* D* N8* I17* R2*NM2* H3* I26* R3* I38* NM4* E8}
V [4]
S* Se12* Se11* E2* N4* P*~{Ne5* I39* H8* N2}*~{H7* I36* R10* NM10* I16*

I24}*~{I110* Ne6* I27* N9* R13* NM12* Ne7* R5* NM8* H5* I37* I18*
I25}*~{Ne5* H7* N2*Ne2* I17* R9* NM3* H9* I310* I36* R10* NM10* I16*
I24}*~{I37* I18* I25* Ne5* H8*N2* I310* Ne1* R17* I13* I22* H4* R2* NM2}
V [3]
H5* I37* Se12* Se11* Ne5*~{Ne7* R5* NM8* I18* I25* E2* N4* P}*~{I18* I25*
E2*N4* P* D* N8* I17* R2* NM2* H3* I26* R3* I38* NM4* E8}
V [2]
S* I37* I18* I25* Se12* Se11* E2* N4* P* Ne5* N2*~{H8* I310* Ne1* R17* I13*
I22*H4* R2* NM2}
V [2]
Ne7* R5* NM8* H5* I37* I18* I25* Se12* Se11* E2* N4* P* Ne2* R17* N3* F
V [1]
H5* I37* I18* I25* Se12* Se11* E2* N4* P* Ne5* D* I35* R4* NM5* E6* N8*
R2*NM2* H3
V [1]
S* I37* I18* I25* Se12* Se11* E2* N4* P* Ne5* N2* H9* Ne1* R17* H4* R2*
NM2*I12* I38* I21* NM11
V [1]
Ne7* R5* NM8* H5* S* I37* I18* I25* Se12* Se11* E2* N4* P* Ne5* I39* H8*
N2*NM9* R12* I19
V [1]
I110* Ne6* I27* N9* R13* NM12* H5* S* I37* Se12* Se11* E2* N4* P* Ne5*
H7* I36*R10* NM10* I16* I24
V [1]
I27* I37* Se12* Se11* P* Ne5* H7* D* N8* I17* NM6* E7* H6* I26* R3* NM9*
I12*I34* R11* E1* N3
V [1]
I110* Ne7* R5* NM8* H5* S* I37* I18* I25* Se12* Se11* E2* N4* P* I39* H8*
N2*NM6* Ne4* I26* R7

CONCEPT FOR CLASS without_compound_AB_2Se_4 :

[5]
Se12* Se11* E2* N4* P* Ne5* H7*~{S* N2* Ne2* I17* R9* NM3* H9* I310* I36*
R10*NM10* I16* I24}*~{I110* Ne6* I27* N9* R13* NM12* H5* S* I37* I36*
R10* NM10*I16* I24}
V [3]
Ne7* R5* NM8* H5* I37* I18* I25* Se12* Se11* E2* N4* P*~{Ne2* R17* N3*
F}*~{I110* Ne6* I27* N9* R13* NM12* S}*~{S* Ne5* I39* H8* N2* NM9* R12*
I19}*~{I110* S*I39* H8* N2* NM6* Ne4* I26* R7}
V [2]
S* Se12* Se11* E2* N4* P* H7* I36* R10* NM10* I16* I24*~{Ne5* N2* Ne2*
I17* R9*NM3* H9* I310}*~{I110* Ne6* I27* N9* R13* NM12* H5* I37* Ne5}
V [2]
S* Se12* Se11* E2* N4* P* Ne5* I39* H8* N2*~{Ne7* R5* NM8* H5* I37* I18*
I25*NM9* R12* I19}
V [2]
Ne7* R5* NM8* H5* I37* I18* I25* Se12* Se11* E2* N4* P* Ne5*~{S* I39* H8*
N2*NM9* R12* I19}
V [1]
I27* Ne7* R5* NM8* H5* I37* I18* I25* Se12* Se11* E2* N4* P* Ne5* H7*
NM9* I12*I34* R11* E1* N3

Feature set III. Predicting Crystal Type for Composition AB_2Se_4

CONCEPT FOR CLASS chalcopyrite :

[9]
S* B2* P*~{B3}*~{B4}
V [5]
S* B2* P* B3* H8* Ne4*~{R4* H10}*~{H7* S5* R5* Ne6* R6* S10}
V [3]
S* B2* P* B3* H8* R7* Ne5* S3*~{Ne7* R1* H6* S9}*~{H7* R6}*~{R5* H1}
V [3]
S* B2* P* B3* Ne4* R4* H10* S10*~{Ne1* R9}*~{S5* Ne6* H4}
V [3]
S* B2* P* B3* H8* R6* Ne5* S9*~{Ne1* R9* S1}*~{R4* S5* Ne6* H4}
V [3]
R7* Ne5* S3*~{S* H8}
V [2]
S* B2* P* B3* H8* Ne4* R4* H10* S5* R5
V [2]
S* B2* P* B3* H8* Ne4* R4* H10* R7* Ne5* S3
V [2]
S* B2* P* B3* Ne6* R6* H5* S6*~{S9}*~{H7* S10}
V [1]
S* B2* P* B3* H8* Ne4* R4* H10* S5* R5* S10
V [1]
S* B2* P* B3* H8* Ne4* S5* R5* R6* Ne5* S9
V [1]
S* B2* P* B3* H8* Ne4* R4* H10* S10* R7* Ne5* S3
V [1]
S* B2* P* B3* Ne4* R4* H10* Ne6* R6* S10* H5* S6
V [1]
S* B2* P* B3* H8* R6* R7* Ne5* S3* S9
V [1]
S* B2* P* B3* H8* Ne6* R6* Ne5* S9* H5* S6
V [1]
S* B2* P* B4* Ne6* R6* Ne7* H5* S6* R2* S7

CONCEPT FOR CLASS spinel :

[1]
B2* P* B3* Ne4* R4* H10* S10* Ne5* H5* R2* S2* D

CONCEPT FOR CLASS $PbGa_2Se_4$:

[6]
B2* B3* H10*~{D* R8* Ne2}*~{S* P* H8* Ne4* R4* R7* Ne5* S3}*~{P* Ne4* R4* S10}*~{S* P* H8* Ne4* R4* S5* R5}*~{S* P* Ne4* R4* Ne1* R9* S6* H9}*~{S* P* Ne4* R4*R5* S1* Ne2* H9}
V [6]
B2* P* B3* R4*~{S9}*~{S* H8* Ne4* H10* R7* Ne5* S3}*~{Ne6* S10}*~{Ne4* H10* S10}*~{S* H8* Ne4* H10* S5* R5}*~{H7* R6}*~{S* Ne4* H10* Ne1* R9* S6* H9}*~{S* Ne4*H10* R5* S1* Ne2* H9}
V [6]
B2* P* B3* Ne4*~{H8* S5* D* R3}*~{S* H8* R4* H10* R7* Ne5* S3}*~{R4* H10* S10}*~{S* H8* R4* H10* S5* R5}*~{H8* S2}*~{S* H8* H7* S5* R5* Ne6* R6*

S10}*~{S*H8* S5* R5* R6* Ne5* S9}*~{S* R4* H10* Ne1* R9* S6* H9}*~{S* R4* H10* R5* S1*Ne2* H9}
V [6]
B2* P* B3* Ne4* R4* H10*~{S}*~{S* H8* R7* Ne5* S3}*~{S10}*~{S10* Ne5}
V [4]
S* B2* P* B3* Ne4* R4* H10* Ne1* R9*~{S6* H9}
V [4]
S* B2* P* B3* Ne4*~{H8}*~{R4* H10* S10}*~{R4* H10}
V [3]
S* B2* P* B3* Ne4* R4* H10* S10* Ne1* R9
V [2]
B2* P* B3* Ne4* R4* H10* R6* Ne5* H6* S6
V [1]
S* B2* P* B3* H8* Ne4* R4* H10* S10* Ne1* R9* S1
V [1]
S* B2* P* B3* H8* Ne4* R4* H10*~{R7* Ne5* S3}*~{S5* R5}
V [1]
S* B2* P* B3* Ne4* R4* H10* S10* S3* Ne1* R9* H9
V [1]
S* B2* P* B3* Ne4* R4* H10* S10* Ne1* R9* S6* H9
V [1]
B2* P* B3* Ne4* R4* H10* R6* S10* Ne5* H6* S6

CONCEPT FOR CLASS olivine :

[3]
B2* P*~{B3}*~{S}*~{Ne4}*~{R6* H6* S6}*~{R1* H4}*~{B4* R5* Ne5}*~{B4* H7* R6* Ne5*Ne7* H5* R2* S7* S4}
V [3]
Ne5*~{R5}*~{B4* R2* D}*~{S3}*~{S* B2* P* B3* H8* R6* S9}*~{B2* P* B3* Ne4}*~{S*B2* P* B3* H8* Ne4* R4* H10* R7* S3}*~{B2* P* B3* Ne4* R4* H10* R6* H6* S6}*~{S*B2* P* B4}*~{B2* B3* H10* R6* S6* D* R8* Ne2}*~{S* B2* P* B3* H8* Ne4* R4* H10*S10* R7* S3}*~{S* B2* P* B3* H8* Ne4* S5* R5* R6* S9}*~{B2* P* B3* Ne4* R4* H10*S10* H5* R2* S2* D}*~{B2* P* B4* H7* R6* Ne7* H5* R2* S7* S4}*~{B2* P* B3* H7*R6* H6* S6}*~{B2* P* B3* H8* R6* H6* S9* R2* S2* D}*~{B2* P* B3* Ne4* R4* H10*R6* S10* H5* S7}*~{B2* B4* Ne4* H10* R6* H5* R2* S2* D}*~{B2* P* B3* H10* R6*H6* S6* D* R8* Ne2}
V [3]
B4*~{D}*~{S* B2* P}*~{Ne7* H5* R2* S7}*~{R5* Ne5}
V [2]
S* B2* P* B4* Ne5* S1
V [2]
H8* Ne5* S3* R1* H4
V [1]
S* B2* P* B4* H7* R5* Ne5* S1* Ne2* H9* S8
V [1]
S* B2* P* B4* H8* Ne5* S3* R1* Ne1* R9* H4* S1
V [1]
B2* P* B4* H8* Ne4* S5* Ne5* S3* R1* H4* D* R3

CONCEPT FOR CLASS $NiCr_2S_4$:

[4]
B4* Ne5* R2* D
V [4]

B4* D*~{B2* P* H8* Ne4* S5* Ne5* S3* R1* H4* R3}
V [2]
B2* P* R1* H4*~{S* B4* H8* Ne5* S3* Ne1* R9* S1}*~{B4* H8* Ne4* S5* Ne5* S3* D*R3}*~{S* B4* Ne5* S3* Ne1* R9* S6* H9}
V [1]
B2* B4* Ne4* H10* R6* Ne5* H5* R2* S2* D

CONCEPT FOR CLASS Th_3P_4 :

[3]
B2* B3* H10* D* R8* Ne2
V [2]
B2* B3* H10* R6* Ne5* S6* D* R8* Ne2
V [1]
S* B2* B3* H8* H10* R7* Ne5* S3* D* R8* Ne2
V [1]
B2* P* B3* H10* R6* Ne5* H6* S6* D* R8* Ne2

CONCEPT FOR CLASS another_structure :

[11]
B2* P* B3*~{H7* R6}*~{R5* Ne5}*~{R4}*~{H8* R6* S9}*~{Ne7* R1* H6* S9}*~{H10* R6*Ne5* H6* S6* D* R8* Ne2}
V [7]
S* B2* P* B3*~{Ne6}*~{Ne4}*~{H8}
V [7]
B2* [illegible]* Ne4*~{B3}*~{S5* R5}*~{B4* H8* S5* Ne5* S3* R1* H4* D* R3}*~{B4* H8* R4*Ne7* H5* R2* S7* S2}
V [3]
S* B2* P* B3* Ne4* R4* H10*~{Ne1* R9}*~{H8* R7* Ne5* S3}*~{H8* S5* R5}*~{Ne6* R6*S10* H5* S6}
V [3]
S* B2* P* B4*~{Ne5}*~{Ne6* R6* Ne7* H5* S6* R2* S7}
V [3]
Ne5* S3*~{H8}*~{R7}*~{S* B2* P* B4* H8* R1* Ne1* R9* H4* S1}*~{S* B2* P* B4* H8*H7* R5* R7* S8}
V [3]
B2* P* B3* H8* Ne4* S5* D* R3
V [2]
B2* P* B3* Ne4* R4* H10* S10*~{Ne5}*~{S* Ne6* R6* H5* S6}*~{S* H8* S5* R5}*~{S*S3* Ne1* R9* H9}*~{S* H8* Ne1* R9* S1}*~{S* Ne1* R9* S6* H9}*~{S3* Ne7* H6* R2}
V [2]
B2* P* B3* Ne4* R4* H10* S10*~{Ne5}*~{S* Ne6* R6* H5* S6}*~{S* H8* S5* R5}*~{S*S3* Ne1* R9* H9}*~{S* H8* Ne1* R9* S1}*~{S* Ne1* R9* S6* H9}*~{S3* Ne7* H6* R2}
V [2]
B2* P* B3* Ne4* R4* H10* S10*~{Ne5}*~{S* Ne6* R6* H5* S6}*~{S* H8* S5* R5}*~{S*S3* Ne1* R9* H9}*~{S* H8* Ne1* R9* S1}*~{S* Ne1* R9* S6* H9}*~{S3* Ne7* H6* R2}
V [2]
B2* P* B3* R4* Ne6* S10*~{S* Ne4* H10* R6* H5* S6}
V [2]
B2* P* B3* R4* H7* Ne6* S9*~{S* R6* H5* S6}*~{S3* Ne7* H6* R2}
V [2]

B2* P* B3* H7* Ne6* R6* S10*~{S}*~{R5* Ne5* H6* S4}
V [2]
S* H8* R7* Ne5* S3*~{B2* P* B3}*~{B2* B3* H10* D* R8* Ne2}*~{B2* P* B4* H7* R5*S8}
V [2]
S* B2* P* B4* Ne5* S3*~{H8* R1* Ne1* R9* H4* S1}*~{H8* H7* R5* R7* S8}
V [2]
S* B2* P* B3* H7* Ne6* Ne1* R9* S6* H9
V [2]
B2* P* B3* H7* Ne6* R6* S10*~{S}*~{S* H5* S6}*~{R5* Ne5* H6* S4}
V [1]
S* B2* P* B3* Ne4* R4* H10* R5* S1* Ne2* H9
V [1]
S* B2* P* B3* Ne4* R4* H10* Ne1* R9* S6* H9*~{S10}
V [1]
S* B2* P* B4* Ne5* S3* R1* Ne1* R9* H4* S6* H9
V [1]
S* B2* P* B3* H8* R6* Ne5* S9* Ne1* R9* S1
V [1]
B2* P* B3* B4* R4* H7* R5* Ne6* S10* Ne5* H6* S9* S4* S8
V [1]
B4* R5* Ne5*~{S* B2* P* H8* H7* S8}*~{B2* P* H5* S7}*~{B2* P* H7* R6* S8}*~{S*B2* P* H7* S1* Ne2* H9* S8}*~{S* B2* P* H8* H7* R7* S3* S8}*~{S* B2* P* H8* Ne4*H7* S5* S8}
V [1]
B4* H7* R5* Ne5* S8*~{S* B2* P* H8}*~{B2* P* R6}*~{S* B2* P* S1* Ne2* H9}
V [1]
B2* P* B4* R5* Ne5*~{H5* S7}*~{H7* R6* S8}*~{S* H7* S1* Ne2* H9* S8}*~{S* H8*H7* R7* S3* S8}*~{S* H8* Ne4* H7* S5* S8}
V [1]
B2* P* B3* H8* Ne4* S5* Ne7* R1* H6* S9* D* R3
V [1]
S* B2* P* B4* H8* Ne4* S5* R5* Ne7* H5* R2* S7
V [1]
S* B2* P* B4* H8* R7* Ne5* S3* Ne7* H5* R2* S7
V [1]
S* B2* P* B3* H8* H7* R6* R7* Ne5* S3
V [1]
S* B2* P* B3* Ne4* R4* H10* S5* Ne6* S10* H4
V [1]
S* B2* P* B3* H7* Ne6* R6* S10* Ne1* R9* S6* H9

CONCEPT FOR CLASS without_compound_AB_2Se_4 :

[11]
R5* Ne5*~{S* B2* P* B3* H8* Ne4* S5* R6* S9}*~{B4}*~{B2* P* B3* B4* R4* H7* Ne6*S10* H6* S9* S4* S8}
V [7]
B2* P* B3* H7* R6*~{Ne6* S10}*~{S* H8* R7* Ne5* S3}
V [6]
B2* P* B3* R5* Ne5*~{S* H8* Ne4* S5* R6* S9}*~{B4* R4* H7* Ne6* S10* H6* S9* S4*S8}
V [6]
B2* P* B3* Ne4*~{}*~{R4* H10}*~{S* H8* R4* H10* R7* Ne5* S3}*~{R4* H10*

R6* Ne5*H6* S6}*~{S* H8* R4* H10* S10* R7* Ne5* S3}*~{S* H8* S5* R5* R6* Ne5* S9}*~{R4*H10* S10* Ne5* H5* R2* S2* D}*~{R4* H10* R6* S10* Ne5* H6* S6}

V [5]

S* B2* P* B3* Ne6*~{R6* H5* S6}*~{H7* Ne1* R9* S6* H9}*~{Ne4* R4* H10* S5* S10*H4}*~{H7* R6* S10* Ne1* R9* S6* H9}

V [4]

B2* P* B3* R4* S9*~{H7* Ne6}

V [4]

S* B2* P* B3* H8*~{R7* Ne5* S3}*~{R6* Ne5* S9}*~{Ne4* R4* H10* S5* R5}*~{R6* R7*Ne5* S3* S9}*~{R6* Ne5* S9* Ne1* R9* S1}*~{Ne4* R4* H10* S10* Ne1* R9* S1}

V [4]

H8* Ne5* S3*~{S* R7}*~{R1* H4}

V [4]

B2* P* B3* H8* R6* S9*~{S* Ne4* S5* R5* Ne5}*~{S* R7* Ne5* S3}*~{S* Ne5* Ne1* R9*S1}*~{S* Ne6* Ne5* H5* S6}

V [3]

B2* P* B3* Ne4* Ne5*~{S* H8* R4* H10* R7* S3}*~{R4* H10* R6* H6* S6}*~{S* H8*R4* H10* S10* R7* S3}*~{S* H8* S5* R5* R6* S9}*~{R4* H10* S10* H5* R2* S2* D}*~{R4* H10* R6* S10* H6* S6}

V [3]

B4* Ne7* H5* R2* S7*~{S* B2* P* Ne6* R6* S6}*~{S* B2* P* H8* R7* Ne5* S3}*~{S*B2* P* H8* Ne4* S5* R5}

V [3]

B2* P* B3* Ne7* R1* H6* S9*~{H8* Ne4* S5* D* R3}

V [3]

B2* P* R6* H6* S6*~{B3* Ne4* R4* H10* Ne5}*~{B3* H10* Ne5* D* R8* Ne2}

V [2]

S* B2* P* B4* H8* H7* R5* Ne5* S8

V [2]

B2* P* Ne4* S5* R5*~{S* B3* H8* R4* H10}*~{S* B3* H8* R6* Ne5* S9}*~{S* B4* H8*Ne7* H5* R2* S7}

V [2]

S* B2* P* B4* Ne5*~{S1}*~{S3}

V [2]

B2* P* B3* H8* Ne4* S2

V [2]

B2* P* B3* Ne4* R4* H10* S10* Ne5*~{S* H8* R7* S3}*~{H5* R2* S2* D}*~{R6* H6*S6}

V [2]

B2* P* B3* R4* H7* R6

V [2]

B2* P* B4* R5* Ne5* H5* S7

V [2]

B2* P* B4* H7* R5* R6* Ne5* S8

V [2]

S* B2* P* B3* Ne6* R6* S9* H5* S6*~{H8* Ne5}

V [2]

S* B2* P* B3* H7* Ne6* R6* S10*~{Ne1* R9* S6* H9}

V [1]

S* B2* P* B4* H8* Ne4* H7* S5* R5* Ne5* S8

V [1]

B2* P* B3* Ne4* R4* H10* R6* S10* Ne5* H5* S7

V [1]
B2* P* B3* R4* H7* Ne6* S3* Ne7* H6* S9* R2
V [1]
S* B2* P* B4* H8* H7* R5* R7* Ne5* S3* S8
V [1]
S* B2* P* B3* R4* H7* Ne6* R6* S9* H5* S6
V [1]
B2* P* B3* H7* R6* Ne5* H6* S6
V [1]
B2* P* B3* H8* R6* Ne5* H6* S9* R2* S2* D
V [1]
S* B2* P* B3* H8* R4* S5* Ne6* R6* Ne5* S9* H4
V [1]
S* B2* P* B3* H8* Ne4* H7* S5* R5* Ne6* R6* S10
V [1]
B2* P* B3* Ne4* R4* H10* S10* S3* Ne7* H6* R2
V [1]
B2* P* B4* H8* Ne4* R4* Ne7* H5* R2* S7* S2
V [1]
B2* P* B4* H7* R6* Ne5* Ne7* H5* R2* S7* S4
V [1]
S* B2* P* B3* H8* R7* Ne5* S3* Ne7* R1* H6* S9
V [1]
S* B2* P* B3* H8* R5* R7* Ne5* S3* H1
V [1]
B2* P* B3* H7* R5* Ne6* R6* S10* Ne5* H6* S4
V [1]
S* B2* P* B3* H7* Ne6* R6* S10* H5* S6

Appendix 2

Logical Expressions for Predicting Crystal Types for Composition ABX_2

Feature Set I

Concept FOR CLASS chalcopyrite :

[38]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10*~{B1* B3}*~{S42* D40* S50}

V [29]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* D40* S50*~{P40}*~{S42}

V [15]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* D40* S50* P40* D30* S40*~{S42}*~{S41* R2}

V [14]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* S41* R2*~{D30* S40* D37* P30* P24* S30}*~{D30* S40* D38* P34}*~{D30* S40* P30* P24* S30* P41}*~{D30* P41* P54* S52* P46*D410}*~{D30* P41* P44}*~{D30* P44* D36}*~{D30* S40* P30* P24* S30* D36}

V [11]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* P54* S52* P46* D410*~{D40* S50* P40* D30* S40* P30* R5* S31}*~{D40* S50* P40* D30* S41* R2* P41}*~{R5* S51}*~{D40* S50* P40* D30* S41* R5*P51}

V [9]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* P46* S51*~{D30* S40* R2* P30* P24* S30}*~{D30* S40* P30* P24* S30* S52* D410* R5* P51}*~{D30* S40* P30* P24* S30* S52*D410* P61* R7* F414* P56* D510* S62}*~{R2* P44* D36}*~{R2* D38* D410* P44* R5}*~{R2* D38* P54* S52* D410* R5}*~{D30* S40* P34* S52* D410* P61* R7* F414*P56* D510* S62}*~{D30* S40* R2* P34* D36}

V [8]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P34*~{S52* P46* D410* P56* S61}*~{P46* S51}*~{S41* R2* D38}*~{P30* S52* P46* D410* R5* S31* P51}*~{S41* S52*P46* D410* R5* P51}*~{S41* S52* P46* D410* P61* R7* F414* P56* D510* S62}

V [8]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P34*~{S52* P46* D410* P56* S61}*~{P46* S51}*~{S41* R2* D38}*~{P30* S52* P46* D410* R5* S31* P51}*~{S41* S52*P46* D410* R5* P51}*~{S41* S52* P46* D410* P61* R7* F414* P56* D510* S62}

V [8]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* R2* P46* D410* R5* S51*~{D38}*~{D30* S40*D37* P30* P24* S30}*~{D30* S40* P30* P24* S30* P41}*~{D30* S40* P30* P24* S30*D38}*~{D30* S40* P30* P24* S30* P31}

V [8]

Appendix 2

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* P34*~{S52* P46* D410* P56*
S61}*~{P46* S51}*~{S41* R2* D38}*~{P30* S52* P46* D410* R5* S31*
P51}*~{S41* S52*P46* D410* R5* P51}*~{S41* S52* P46* D410* P61* R7* F414*
P56* D510* S62}

V [8]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* S52* P46* D410* R5* S51*~{D40* S50* P40* D30* S40* P30*
P24*S30}*~{P54}*~{D40* S50* P40* D30* S40* P30* P24* S30* P61* R7* F414*
P56*D510* S62}

V [7]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* R2* D36*~{D40* S50* P44}*~{D40* S50* P40* D30* S40*
S41*P30* P24* S30}*~{D40* S50* P40* D30* S40* P34* P46* S51}*~{D40* S50*
P40* D30*S40* P34* S52* P46* D410* P56* S61}

V [7]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D36*~{D40* S50* R2* P44}*~{D40* S50* P40* D30* S41*
R2* P44}*~{D40* S50* P40* D30* S40* S41* R2* P30* P24* S30}*~{D40* S50*
P40* D30* S40*R2* P34* P46* S51}*~{D40* S50* P40* D30* S40* R2* P34* S52*
P46* D410* P56*S61}

V [5]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 S42* D40* S50* P40* B2*~{D30* S40* P34}*~{D30* S40* R2* P30* P24*
S30*R3}

V [4]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* S52* P46* D410* R5*~{P30*
S31}*~{P30}*~{P30* P24* S30* S51* P51}*~{P51}*~{S41* P30* P24* S30*
P51}*~{P30* P54*S31* P51}*~{P30* P44* S31* P51}*~{P30* S30* P44* P51* R3*
S21* P20}

V [4]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 S42* D40* S50* P40* R2* B2* R3*~{D30* S40* P30* P24* S30}

V [3]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* P54* S52* P46* D410*~{P30* R5*
S31}

V [3]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S41* S52* P46* D410*~{R2* P41*
P54}*~{P54* R5* P51}*~{S40* P34* R5* P51}*~{S40* P34* P61* R7* F414* P56*
D510* S62}*~{S40* P30* P24* S30* R5* P51}*~{P44* R5* P51}*~{S40* P30* P24*
S30* P61* R7*F414* P56* D510* S62}

V [3]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* R2* P46* D410* R5* S51*
P31*~{P30*P24* S30}

V [3]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 S42* D40* S50* P40* D30* S40* R2* P31* B2* R3

V [3]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 S42* D40* S50* R2* P41* P54* S52* P46* D410* B2

V [2]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* S41* R2* P31
V [2]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* R2* P46* D410* D36* R5* S51
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* P30* S30* P54* S52* P46* D410*
R5*P51* R3* S21* P20
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* D40* S50* P40* D30* S40* S41* R2* P34* P31
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* S41* R2* P44* P31
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* S41* R2* P54* S52* P46* D410*
P31
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* S41* R2* P34* P41
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* S41* R2* P41* P44*~{D30}
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* S41* R2* P41* P54* S52* P46* D410*~{D30}
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* S41* R2* P34* S52* P46* D410*
R5*P51
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* S41* R2* S52* P46* D410* P44* R5* P51
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* S41* R2* P54* S52* P46* D410* R5* P51
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* S41* R2* P34* S52* P46* D410*
P61*R7* F414* P56* D510* S62
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* S41* R2* S52* P46* D410* P44* P61* R7*
F414*P56* D510* S62
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* S41* R2* P54* S52* P46* D410* P61* R7*
F414*P56* D510* S62
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* S41* R2* P34* D36

V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* S41* R2* P44* D36*~{D30}
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* S41* R2* P54* S52* P46* D410* D36
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* R2* P34* P46* D410* R5* S51*
P31
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* R2* P46* D410* P44* R5* S51*
P31
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* R2* P54* S52* P46* D410* R5*
S51*P31
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* R2* P34* P41* P46* D410* R5*
S51
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* R2* P41* P46* D410* P44* R5* S51
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* R2* P41* P54* S52* P46* D410* R5* S51
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* P34* S52* P46* D410* R5* S51*
P51
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* S52* P46* D410* P44* R5* S51* P51
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* S52* P46* D410* P44* R5* S51* P61* R7* F414*
P56*D510* S62
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30*~{}*~{D37*
P46*D410* R5* S51}*~{P41* P46* D410* R5* S51}*~{D38* P46* D410* R5*
S51}*~{P46*D410* R5* S51* P31}
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30* P46* D410*
R5*S51*~{D37}*~{P41}*~{D38}*~{P31}
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30* P46* D410*
D36*R5* S51
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-

R10 B1* B3* S42* D40* S50* P40* D30* S40* R2* P34* P46* D410* D36* R5* S51

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* S42* D40* S50* P40* D30* S40* R2* P34* P31* B2* R3

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* S42* D40* S50* P40* D30* S40* R2* P44* P31* B2* R3

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* S42* D40* S50* P40* D30* S40* R2* P54* S52* P46* D410* P31* B2* R3

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* S42* D40* S50* P40* P54* S52* P46* D410* P61* R7* F414* P56* D510* S62*B2* R3

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* P54* S52* P46* D410* R5* S51* P51

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* P54* S52* P46* D410* R5* S51* P61* R7* F414* P56* D510* S62

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* R2* P46* D410* P44* D36* R5* S51

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* R2* P54* S52* P46* D410* D36* R5* S51

Concept FOR CLASS b-$NaFeO_2$:

[5]

S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1* B3*D40* S50* P40* P30*~{P36* D30* S40}*~{P36* S42* D30* S40}*~{D30* S40* R2* P24*S30* P31* R3* S21* P20}

V [5]

D30* S40*~{P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70*B2-* R10}*~{D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60*S70* B2-* R10* B1* B3* D40* S50* P40}*~{P31}

V [5]

P30* S30*~{P24}*~{D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60*D60* S70* B2-* R10* S42* D40* S50* P40* D30* S40* R2* P24* B2* R3}*~{S12* S22*P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1* B3* D40* S50*P40* R3* S21* P20}*~{D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60*P60* D60* S70* B2-* R10* B1* B3* S42* D40* S50* P40* D30* S40* P54* S52* P46*D410* R5* P51* R3* S21* P20}*~{D310* P36* S12* S22* P26* S32* F40* P50* D50*F50* S60* P60* D60* S70* B2-* R10* B1* B3* S42* D40* S50* P40* D30* S40* P24*S52* P46* D410* R5* P51* R3* S21* P20}

V [3]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30*~{P24* S30}*~{R5* S31}*~{S30*P54* S52* P46* D410* R5* P51* R3* S21* P20}

V [3]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-

R10 B1* B3* S42* D40* S50* P40* D30* S40*~{P46* S51}*~{S52* P46* D410* P56*S61}*~{S41* R2* D37* P30* P24* S30}*~{S41* R2* D38* P34}*~{S41* R2* P44* P31}*~{S41* R2* P30* P24* S30* P41}*~{S41* R2* P34* P41}*~{S41* R2* P34* D36}*~{S41* R2* P34* S52* P46* D410* R5* P51}*~{S41* R2* P34* S52* P46* D410* P61*R7* F414* P56* D510* S62}*~{S41* R2* P54* S52* P46* D410* P31}*~{S41* R2* P30*P24* S30* D36}*~{P30* S30* P54* S52* P46* D410* R5* P51* R3* S21* P20}*~{P30*P34* S52* P46* D410* R5* S31* P51}*~{S41* P34* S52* P46* D410* R5* P51}*~{S41* P34* S52* P46* D410* P61* R7* F414* P56* D510* S62}*~{S41* P30* P24* S30*S52* P46* D410* R5* P51}*~{P30* P54* S52* P46* D410* R5* S31* P51}*~{P30* S52*P46* D410* P44* R5* S31* P51}*~{S41* P30* P24* S30* S52* P46* D410* P61* R7*F414* P56* D510* S62}*~{P30* P24* S30* S52* P46* D410* R5* P51* R3* S21* P20}*~{P30* P24* S30* S52* P46* D410* R5* S31* P51}*~{P30* P24* S30* S52* P46*D410* R5* S31* P61* R7* F414* P56* D510* S62}*~{R2* P30* P44* R5* S31* P31}*~{R2* P30* P54* S52* P46* D410* R5* S31* P31}*~{R2* P30* P41* P54* S52* P46*D410* R5* S31}*~{P30* P24* S30* S52* P46* D410* P61* R7* F414* P56* D510* S62*R3* S21* P20}*~{R2* P30* D38* P44* R5* S31}

V [3]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40*~{P30* P24* S30}*~{}*~{S52* P46*D410}*~{P30* P24* S30}*~{P30* R5* S31}*~{P30* S30* P54* S52* P46* D410* R5*P51* R3* S21* P20}

V [3]

S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1* B3*D40* S50* P40* R2* P30* P24* S30*~{P36* S42* D30* S40}*~{P36* D30* S40}*~{D30* S40* P31* R3* S21* P20}*~{P36* S42* D30* S40* D37* R5* S31}*~{P36* S42*D30* S40* D36* R5* S31}*~{P36* S42* D30* S40* D38* R5* S31}

V [2]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30* P24* S30* P41*~{S41* R2}*~{R2* P46* D410* R5* S51}*~{R2* P46* S51}

V [1]

S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1* B3*D40* S50* P40* D30* S40* R2* P30* S30* P34* P31* R3* S21* P20

V [1]

S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1* B3*D40* S50* P40* D30* S40* R2* P30* S30* P31* R3* S21* P20*~{P24}

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30* P41* R3* S21*P20

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30* S30* S52* P46* D410* P44* R5*P51* R3* S21* P20

V [1]

S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1* B3*D40* S50* P40* D30* S40* R2* P30* P24* S30* R5* S31* P31

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30* P41* R5* S31

V [1]

P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1*B3* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30* R5* S31*~{D37}*~{D36}*~{D38}

Concept FOR CLASS a-$NaFeO_2$:

[22]
P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1*B3* D40* S50* P40* D30* S40* P30*~{D310* S42}*~{D310* S42* S52* P46* D410* R5}*~{R2* P24* S30}

V [21]
S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1* B3*D40* S50* P40* P30* P24* S30*~{R2}*~{D310* P36* S42* D30* S40}*~{D310* P36*S42* D30* S40* S52* P46* D410* P61* R7* F414* P56* D510* S62* R3* S21* P20}

V [20]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* D40* S50* P40*~{S42}*~{D30* S40}

V [20]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3*~{D40* S50}*~{S42}

V [19]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50*~{P40}*~{P40* R2* P46* D410* R5* S51}*~{P44}*~{P40* D30* S40* R2* P34* P41* P46* D410* R5* S51}*~{P40* D30* S40* P34* S52*P46* D410* R5* S5[illegible] P51}*~{S52* P46* D410* P44* R5* S51* P51}*~{R2* P41* P46*D410* P44* R5* S51}*~{R2* P41* P54* S52* P46* D410* R5* S51}

V [15]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30* P24* S30*~{R2}*~{S52* P46*D410}*~{S52* P46* D410* R5* P51* R3* S21* P20}

V [11]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* S52* P46* D410*~{P56* S61}*~{R5}*~{P61* R7* F414* P56* D510* S62}*~{S41* R2* P54* P31}*~{S41* P34* P61* R7*F414* P56* D510* S62}*~{P30* P24* S30* P61* R7* F414* P56* D510* S62* R3* S21*P20}

V [7]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P46* S51*~{R2* P30* P24* S30}*~{P34}*~{R2* D410* P44* R5* P31}*~{R2* P54* S52* D410* R5* P31}*~{R2* P30* P24*S30* P41}

V [5]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30* P24* S30* S52* P46* D410* P61*R7* F414* P56* D510* S62*~{R3* S21* P20}

V [4]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30* R5* S31*~{R2}*~{P54* S52* P46*D410* P51}

V [4]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* D40* S50* P40* D30* S40* S41* R2*~{S42* P31}*~{S42* D38*

P34}*~{S42* P34* P41}*~{S42* P34* D36}*~{S42* P34* S52* P46* D410* R5* P51}*~{S42* P34* S52* P46* D410* P61* R7* F414* P56* D510* S62}*~{P34* P31}
V [3]
P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1*B3* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30* D38
V [3]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30* P24* S30* S52* P46* D410* R5*S51
V [3]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* R2* D38* P46* D410* R5* S51
V [2]
D30* S40* P31*~{P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60*S70* B2-* R10* B1* B3* D40* S50* P40* R2* P30* P24* S30}*~{D310* P36* S12*S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* S42* D40*S50* P40* R2* B2* R3}*~{D310* P36* S12* S22* P26* S32* F40* P50* D50* F50*S60* P60* D60* S70* B2-* R10* B1* B3* S42* D40* S50* P40* R2* P30* R5* S31}*~{D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* S41* R2* P44}*~{D310* P36* S12* S22* P26*S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1* B3* S42* D40* S50*P40* S41* R2* P54* S52* P46* D410}*~{D310* P36* S12* S22* P26* S32* F40* P50*D50* F50* S60* P60* D60* S70* B2-* R10* B1* B3* S42* D40* S50* P40* R2* P34*P46* D410* R5* S51}*~{D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60*P60* D60* S70* B2-* R10* B1* B3* S42* D40* S50* P40* R2* P46* D410* P44* R5*S51}*~{D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70*B2-* R10* B1* B3* S42* D40* S50* P40* R2* P54* S52* P46* D410* R5* S51}*~{D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* D40* S50* P40* S41* R2* P34}*~{S12* S22* P26* S32* F40* P50* D50*F50* S60* P60* D60* S70* B2-* R10* B1* B3* D40* S50* P40* R2* P30* P24* S30*R5* S31}*~{S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* D40* S50* P40* R2* P30* S30* R3* S21* P20}
V [2]
S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1* B3*D40* S50* P40* R2* P30* S30* R3* S21* P20*~{D30* S40* P31}*~{D310* P36* S42*D30* S40* P24* P41}*~{P36* S42* D30* S40* P24* D36}
V [2]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30* P24* S30* S52* P46* D410* R5*S51* P51
V [2]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30* P24* S30* S52* P46* D410* S51*P61* R7* F414* P56* D510* S62
V [1]
S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1* B3*D40* S50* P40* D30* S40* R2* P30* P24* S30* P31* R3* S21* P20
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30* P34* S52* P46* D410* R5* S31*P51
V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30* S52* P46* D410* P44* R5* S31*P51

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30* P24* S30* S52* P46* D410* R5*S31* P51

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30* P24* S30* S52* P46* D410* R5*S31* P61* R7* F414* P56* D510* S62

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* S41* P30* P24* S30* S52* P46* D410*R5* P51

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* S41* P30* P24* S30* S52* P46* D410*P61* R7* F414* P56* D510* S62

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30* P24* S30* S52* P46* D410* P61*R7* F414* P56* D510* S62* S61

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* S41* R2* P30* P24* S30* P41

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* S41* R2* P30* P24* S30* D36

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* S41* R2* D37* P30* P24* S30

V [1]

P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1*B3* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30* D38* R3* S21* P20

V [1]

P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1*B3* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30* D36* R5* S31

V [1]

P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1*B3* S42* D40* S50* P40* D30* S40* R2* D37* P30* P24* S30* R5* S31

V [1]

P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1*B3* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30* D38* R5* S31

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* D40* S50* P40* D30* S40* S41* R2* P30* P24* S30* P31

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30* P41* P46* D410*R5* S51

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30* P24* S30* S52* P46* D410*

R5*S51* P61* R7* F414* P56* D510* S62
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* R2* D37* P30* P24* S30* P46*
D410*R5* S51
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30* D38* P46*
D410*R5* S51
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* R2* D38* P46* D410* P44* R5* S51
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* R2* D38* P54* S52* P46* D410* R5* S51
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* P54* S52* P46* D410* R5* S51*~{P61* R7* F414* P56*
D510*S62}*~{P51}*~{D40* S50* P40* D30* S40* R2* P31}*~{D40* S50* P40* R2*
D36}*~{D40* S50* R2* P41}

Concept FOR CLASS TlSe:

[6]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 S42* D40* S50*~{B1* B3* P40}*~{B2}*~{B1* B3* S52* P46* D410* P44*
R5*S51* P51}*~{B1* B3* S52* P46* D410* P44* R5* S51* P61* R7* F414* P56*
D510*S62}*~{B1* B3* R2* P41* P46* D410* P44* R5* S51}*~{B1* B3* R2* P41*
P54* S52*P46* D410* R5* S51}
V [5]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30*~{S52* P46* D410}*~{P44}*~{P46*
D410* R5}*~{S40}
V [3]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* R2* P30* R5* S31*~{P24* S30*
P41}*~{D38* P44}
V [3]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* P30* P54* S52* P46* D410* R5*
S31
V [3]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* P30* S52* P46* D410* R5*
S31*~{P34* P51}*~{P44* P51}*~{P24* S30* P51}*~{P24* S30* P61* R7* F414*
P56* D510*S62}
V [3]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* P30* S52* P46* D410* R5*~{P24*
S30*S51* P51}*~{S30* P54* P51* R3* S21* P20}*~{P34* S31* P51}*~{P24* S30*
S51*P61* R7* F414* P56* D510* S62}*~{S41* P24* S30* P51}*~{P44* S31*
P51}*~{S30*P44* P51* R3* S21* P20}*~{P24* S30* P51* R3* S21* P20}*~{P24*
S30* S31* P51}*~{P24* S30* S31* P61* R7* F414* P56* D510* S62}
V [2]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-

R10 B1* B3* S42* D40* S50* P40* D30* S40* R2* P30* R5* S31* P31
V [2]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S52* P46* D410* R5* P51*~{S40}*~{S41*P44}
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* R2* P30* P44* R5* S31* P31
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* R2* P30* P54* S52* P46* D410* R5*S31* P31
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* R2* P30* P41* P54* S52* P46* D410*R5* S31
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30* P54* S52* P46* D410* R5* S31*P51
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S41* P54* S52* P46* D410* R5* P51
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* S42* D40* S50* S52* P46* D410* P44* R5* P61* R7* F414* P56* D510* S62*B2

Concept FOR CLASS a-$LiFeO_2$:

[3]
S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1* B3*D40* S50* P40* P30* S30* R3* S21* P20*~{R2}*~{D310* P36* S42* D30* S40* P54*S52* P46* D410* R5* P51}*~{D310* P36* S42* D30* S40* S52* P46* D410* P44* R5*P51}
V [3]
P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1*B3* S42* D40* S50* P40* D30* S40* P30*~{D310* P24* S30}*~{D310* P24* S30* S52*P46* D410* P61* R7* F414* P56* D510* S62}*~{D310* R2* P24* S30}*~{D310* R5*S31}*~{D310* S52* P46* D410* R5* S31}*~{D310* P24* S30* S52* P46* D410* R5*S51}*~{R2* D37* P24* S30}*~{D310* S41* R2* D37* P24* S30}*~{D310* S41* R2*P24* S30* P41}*~{D310* S41* R2* P24* S30* D36}*~{D310* R2* P24* S30}*~{S41*R2* P24* S30* D36}*~{D310* S30* P54* S52* P46* D410* R5* P51* R3* S21* P20}*~{D310* R2* P24* S30* P46* D410* D36* R5* S51}*~{D310* S41* P24* S30* S52*P46* D410* R5* P51}*~{D310* S30* S52* P46* D410* P44* R5* P51* R3* S21* P20}*~{D310* S41* P24* S30* S52* P46* D410* P61* R7* F414* P56* D510* S62}*~{R2*P24* S30* R5* S31}*~{R2* P24* S30* D36* R5* S31}*~{R2* P24* S30* D38* R5* S31}*~{R2* P24* S30* D38* R3* S21* P20}
V [2]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30* P24* S30* S52* P46* D410*~{R5* S51* P51}*~{S51* P61* R7* F414* P56* D510* S62}*~{S41* R5* P51}*~{S41*P61* R7* F414* P56* D510* S62}*~{R5* S31* P51}*~{R5* S31* P61*

R7* F414* P56*D510* S62}*~{P61* R7* F414* P56* D510* S62* S61}*~{R2* P56* S61* P31}
V [2]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30* P24* S30*~{}*~{S52* P46* D410*P61* R7* F414* P56* D510* S62}*~{S52* P46* D410* R5* S51}*~{S41* R2* D37}*~{S41* R2* P41}*~{S41* R2* D36}*~{R2}*~{S41* S52* P46* D410* R5* P51}*~{S41*S52* P46* D410* P61* R7* F414* P56* D510* S62}
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30* P24* S30* S52* P46* D410* R5*P51* R3* S21* P20
V [1]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P30* P24* S30* S52* P46* D410* P61*R7* F414* P56* D510* S62* R3* S21* P20
V [1]
P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1*B3* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30* D36* R3* S21* P20
V [1]
P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1*B3* S42* D40* S50* P40* D30* S40* R2* P30* P24*
S30*~{D310}*~{D38}*~{D37}*~{D310* S41* D37}*~{D310* S41* P41}*~{D310* S41* D36}*~{D310}*~{S41* D36}*~{D310* P46* D410* D36* R5* S51}*~{R5* S31}*~{D36* R5* S31}*~{D38* R5* S31}*~{D38* R3* S21* P20}
V [1]
P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1*B3* D40* S50* P40* D30* S40* R2* P30* P24* S30*~{D310*
S42}*~{P31}*~{S42* D37}*~{D310* S42* S41* D37}*~{D310* S42* S41* P41}*~{D310* S42* S41* D36}*~{D310*S42}*~{S42* S41* D36}*~{D310* S42* P46* D410* D36* R5* S51}*~{S42* D36* R5*S31}*~{S42* D38* R5* S31}*~{S42* D38* R3* S21* P20}
V [1]
P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1*B3* S42* D40* S50* P40* D30* S40* R2* P30* P24*
S30*~{D310}*~{D37}*~{D310*S41* D37}*~{D310* S41* P41}*~{D310* S41* D36}*~{D310}*~{S41* D36}*~{D310* P46*D410* D36* R5* S51}*~{D36* R5* S31}*~{D38* R5* S31}*~{D38* R3* S21* P20}
V [1]
P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1*B3* S42* D40* S50* P40* D30* S40* R2* P30* P24*
S30*~{D310}*~{D37}*~{S41* D36}*~{D310* P46* D410* D36* R5* S51}*~{D36* R5* S31}*~{D38* R5* S31}*~{D38* R3*S21* P20}
V [1]
P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1*B3* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30* D36*~{S41}*~{D310* P46*D410* R5* S51}*~{R5* S31}

Concept FOR CLASS another structure :

[21]
P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10*D30* S40*~{B1* B3* D40* S50* P40* P30}*~{S42* D40* S50}*~{D310* B1* B3* D40*S50* P40* S41* R2* P34* P31}
V [20]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40*~{P46* S51}*~{D30* S40*
P34}*~{D30}*~{D30*S40}*~{D30* S40* P30}*~{R2* D38* P46* D410* R5*
S51}*~{S41* R2* P41* P54* S52*P46* D410}*~{S41* R2* P41* P44}*~{S41* R2*
P44* D36}*~{S41* R2* P54* S52* P46*D410* D36}*~{S41* R2* S52* P46* D410*
P44* R5* P51}*~{D30* S40* S41* R2* P34*S52* P46* D410* R5* P51}*~{S41*
R2* P54* S52* P46* D410* R5* P51}*~{S41* R2*S52* P46* D410* P44* P61* R7*
F414* P56* D510* S62}*~{D30* S40* S41* R2* P34*S52* P46* D410* P61* R7*
F414* P56* D510* S62}*~{S41* R2* P54* S52* P46* D410*P61* R7* F414* P56*
D510* S62}
V [20]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40*~{P46* S51}*~{D30* S40*
P34}*~{D30}*~{D30*S40}*~{D30* S40* P30}*~{D30* S40}*~{R2* D38* P46* D410*
R5* S51}*~{S41* R2*P41* P54* S52* P46* D410}*~{S41* R2* P41* P44}*~{S41*
R2* P44* D36}*~{S41* R2*P54* S52* P46* D410* D36}*~{S41* R2* S52* P46*
D410* P44* R5* P51}*~{D30* S40*S41* R2* P34* S52* P46* D410* R5*
P51}*~{S41* R2* P54* S52* P46* D410* R5*P51}*~{S41* R2* S52* P46* D410*
P44* P61* R7* F414* P56* D510* S62}*~{D30*S40* S41* R2* P34* S52* P46*
D410* P61* R7* F414* P56* D510* S62}*~{S41* R2*P54* S52* P46* D410* P61*
R7* F414* P56* D510* S62}
V [20]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42*~{P54* S52* P46* D410}*~{D40* S50* P40* P46* S51}*~{D40*
S50*P40* D30* S40* P[illegible]}*~{S52* P46* D410* R5* S51}*~{D36}*~{D40* S50* P40*
D30}*~{D40* S50* P40* D30* S40}*~{D40* S50* P40* D30* S40* P30}*~{D40*
S50* P40*D30* S40}*~{D40* S50* P40* R2* D38* P46* D410* R5* S51}*~{D40*
S50* P40* S41*R2* P41* P54* S52* P46* D410}*~{D40* S50* P40* S41* R2* P41*
P44}*~{D40* S50*P40* S41* R2* P44* D36}*~{D40* S50* P40* S41* R2* P54*
S52* P46* D410* D36}*~{D40* S50* P40* S41* R2* S52* P46* D410* P44* R5*
P51}*~{D40* S50* P40* D30*S40* S41* R2* P34* S52* P46* D410* R5*
P51}*~{D40* S50* P40* S41* R2* P54*S52* P46* D410* R5* P51}*~{D40* S50*
P40* S41* R2* S52* P46* D410* P44* P61*R7* F414* P56* D510* S62}*~{D40*
S50* P40* D30* S40* S41* R2* P34* S52* P46*D410* P61* R7* F414* P56* D510*
S62}*~{D40* S50* P40* S41* R2* P54* S52* P46*D410* P61* R7* F414* P56*
D510* S62}*~{D40* S50* R2* P41* P46* D410* P44* R5*S51}
V [20]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40*~{S41* R2}*~{P46* S51}*~{D30* S40*
P34}*~{D30* S40* P34}*~{R2* P46* D410* R5* S51}*~{D30}*~{D30* S40}*~{D30*
S40* P30}*~{D30* S40}*~{R2* D38* P46* D410* R5* S51}*~{D30* S40* R2* P46*
D410* R5*S51* P31}*~{S41* R2* P41* P54* S52* P46* D410}*~{S41* R2* P41*
P44}*~{S41* R2*P44* D36}*~{S41* R2* P54* S52* P46* D410* D36}*~{S41* R2*
S52* P46* D410* P44*R5* P51}*~{D30* S40* S41* R2* P34* S52* P46* D410*
R5* P51}*~{S41* R2* P54*S52* P46* D410* R5* P51}*~{S41* R2* S52* P46*
D410* P44* P61* R7* F414* P56*D510* S62}*~{D30* S40* S41* R2* P34* S52*
P46* D410* P61* R7* F414* P56* D510*S62}*~{S41* R2* P54* S52* P46* D410*
P61* R7* F414* P56* D510* S62}*~{D30*S40* R2* P34* P46* D410* R5* S51*
P31}*~{D30* S40* R2* P34* P41* P46* D410*R5* S51}*~{D30* S40* R2* P34*
P46* D410* D36* R5* S51}
V [14]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40*~{P34}*~{}*~{S41* R2* P34* S52*
P46*D410* R5* P51}*~{S41* R2* P34* S52* P46* D410* P61* R7* F414* P56*

D510* S62}
V [14]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40*~{P34}*~{}*~{P54* S52* P46* D410}*~{R2* P46* D410* R5* S51* P31}*~{R2* P46* D410* D36* R5* S51}*~{S41* R2* P31}
V [13]
P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10*S42* D40* S50* D30* S40* P34*~{D310* B1* B3* P40}*~{D310* B1* B3* P40* S41*R2* D36}*~{D310* P40* R2* P31* B2* R3}*~{D310* P40* S52* P46* D410* P61* R7*F414* P56* D510* S62* B2* R3}
V [10]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S52* P46* D410*~{S41}*~{S40* P30* P24*S30* S51* P61* R7* F414* P56* D510* S62}*~{S40* P30* P24* S30}*~{S40* S41* R2*P34* P61* R7* F414* P56* D510* S62}*~{S40* P30* S30* P54* R5* P51* R3* S21*P20}*~{S40* R2* P54* R5* S51* P31}*~{S40* P34* R5* S51* P51}*~{S40* P30* P34*R5* S31* P51}*~{S40* P30* P54* R5* S31* P51}*~{S40* P30* P44* R5* S31* P51}*~{S40* P30* S30* P44* R5* P51* R3* S21* P20}*~{S40* S41* P30* P24* S30* P61*R7* F414* P56* D510* S62}*~{S40* P30* P24* S30* R5* S31* P61* R7* F414* P56*D510* S62}*~{S40* R2* P30* P54* R5* S31* P31}*~{S40* R2* P30* P41* P54* R5*S31}*~{S40* P30* P24* S30* P61* R7* F414* P56* D510* S62* R3* S21* P20}*~{S40* P30* P24* S30* P61* R7* F414* P56* D510* S62* S61}
V [7]
P30* P24* S30*~{S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70*B2-* R10* B1* B3* D40* S50* P40}*~{D310* P36* S12* S22* P26* S32* F40* P50*D50* F50* S60* P60* D60* S70* B2-* R10* B1* B3* S42* D40* S50* P40* D30* S40*S52* P46* D410* P61* R7* F414* P56* D510* S62}*~{D310* P36* S12* S22* P26*S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* S42* D40* S50* P40*D30* S40* R2* B2* R3}*~{D310* P36* S12* S22* P26* S32* F40* P50* D50* F50*S60* P60* D60* S70* B2-* R10* B1* B3* S42* D40* S50* P40* D30* S40}*~{D310*P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1*B3* S42* D40* S50* P40* D30* S40* P41}*~{D310* P36* S12* S22* P26* S32* F40*P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1* B3* S42* D40* S50* P40* D30*S40* R2* P46* D410* D36* R5* S51}*~{D310* P36* S12* S22* P26* S32* F40* P50*D50* F50* S60* P60* D60* S70* B2-* R10* B1* B3* S42* D40* S50* P40* D30* S40*S41* S52* P46* D410* P61* R7* F414* P56* D510* S62}*~{D310* P36* S12* S22*P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1* B3* S42* D40*S50* P40* D30* S40* S52* P46* D410* R5* S31* P51}*~{D310* P36* S12* S22* P26*S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1* B3* S42* D40* S50*P40* D30* S40* S52* P46* D410* R5* S31* P61* R7* F414* P56* D510* S62}
V [6]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P44*~{P40* D30* S40* S41* R2* P31}*~{P40* S41* R2*P41}*~{P40* S41* R2* D36}*~{P40* S41* R2* S52* P46* D410* R5* P51}*~{P40* S41*R2* S52* P46* D410* P61* R7* F414* P56* D510* S62}*~{P40* D30* S40* R2* P46*D410* R5* S51* P31}*~{P40* R2* D38* P46* D410* R5* S51}*~{P40* R2* P46* D410*D36* R5* S51}*~{S52* P46* D410* R5* S51* P51}*~{S52* P46* D410* R5* S51* P61*R7* F414* P56* D510* S62}*~{P40* D30* S40* P30* S52* P46* D410* R5* S31* P51}*~{P40* D30* S40* P30* S30* S52* P46* D410* R5* P51* R3* S21* P20}*~{R2* P41*P46* D410* R5* S51}*~{P40* D30* S40* R2* P30* R5* S31* P31}

V [5]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* S52* P46* D410* P56*
S61*~{P30*P24* S30* P61* R7* F414* D510* S62}
V [4]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* P44*~{S40* S41* R2* P31}*~{S40* R2*
P46*D410* R5* S51* P31}*~{S40* P30* S52* P46* D410* R5* S31* P51}*~{S40*
P30* S30*S52* P46* D410* R5* P51* R3* S21* P20}*~{S40* R2* P30* R5* S31*
P31}
V [4]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* P30* P24* S30*~{S52* P46*
D410*P61* R7* F414* P56* D510* S62}*~{}*~{P41}*~{S41* S52* P46* D410* P61*
R7*F414* P56* D510* S62}*~{S52* P46* D410* R5* S31* P51}*~{S52* P46*
D410* R5*S31* P61* R7* F414* P56* D510* S62}
V [4]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30*~{S41*
D37}*~{S41* P41}*~{S41* D36}*~{D37* P46* D410* R5* S51}*~{P41* P46* D410*
R5* S51}*~{D38* P46* D410* R5* S51}*~{P46* D410* D36* R5* S51}*~{P41* R3*
S21* P20}*~{P41* R5* S31}
V [4]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* P46* D410* R5*~{S52* P51}*~{S41*
P54*S52* P51}*~{S40* R2* P34* S51* P31}*~{S40* R2* P44* S51* P31}*~{S40*
R2* P54*S52* S51* P31}*~{S40* R2* P34* P41* S51}*~{S40* R2* P34* D36*
S51}*~{S40* R2*D37* P30* P24* S30* S51}*~{S40* R2* P30* P24* S30* P41*
S51}*~{S40* R2* P30*P24* S30* D38* S51}*~{S40* R2* P30* P24* S30* D36*
S51}*~{S40* P30* P24* S30*S52* S51* P61* R7* F414* P56* D510* S62}*~{S40*
P30* P24* S30* S52* S31* P61*R7* F414* P56* D510* S62}*~{S40* R2* P30*
P54* S52* S31* P31}*~{S40* R2* P30*P41* P54* S52* S31}
V [4]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* P34* S52* P46* D410* P56* S61
V [3]
P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10*
B1*B3* D40* S50* P40* D30* S40* R2* P30* P24* S30* P31*~{D310* S41}
V [3]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* S52* P46* D410* P61* R7* F414*
P56*D510* S62*~{P30* P24* S30* S51}*~{S41* R2* P34}*~{S41* P30* P24*
S30}*~{P30*P24* S30* R5* S31}*~{P30* P24* S30* R3* S21* P20}*~{P30* P24*
S30* S61}
V [3]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 B1* B3* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30* P46*
S51*~{D37*D410* R5}*~{P41* D410* R5}*~{D38* D410* R5}*~{D410* D36* R5}
V [3]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-
R10 S42* D40* S50* P40* D30* S40* P34* B2*~{R2* P31* R3}*~{S52* P46*
D410*P61* R7* F414* P56* D510* S62* R3}
V [3]
D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-

R10 S42* D40* S50* B2*~{P40}*~{P40* R3}*~{R2* P41* P54* S52* P46* D410}*~{S52* P46* D410* P61* R7* F414* P56* D510* S62}*~{S52* P46* D410* P44* R5* P61*R7* F414* P56* D510* S62}

V [3]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* R2* P44* D36*~{P40* S41}*~{P40* P46* D410* R5*S51}

V [2]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* S52* P46* D410* R5* P51*~{P30* P24*S30* S51}*~{S41* R2* P34}*~{P30* S30* P54* R3* S21* P20}*~{P34* S51}*~{P30*P34* S31}*~{S41* P30* P24* S30}*~{P30* P54* S31}*~{P30* P44* S31}*~{P30* S30*P44* R3* S21* P20}*~{P30* P24* S30* R3* S21* P20}*~{P30* P24* S30* S31}

V [2]

P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1*B3* S42* D40* S50* P40* D30* S40* R2* D37* P30* P24* S30*~{D310* S41}*~{D310*P46* D410* R5* S51}*~{R5* S31}

V [2]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P34* P46* S51*~{R2* D410* R5* P31}*~{R2* P41* D410* R5}*~{S52* D410* R5* P51}*~{R2* D410* D36* R5}

V [2]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* S42* D40* S50* P40* D30* S40* P34* S52* P46* D410* P61* R7* F414* P56*D510* S62* B2*~{R3}

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* R2* P30* D38* P44* R5* S31

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* S41* P34* S52* P46* D410* R5* P51*~{R2}

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* S41* P34* S52* P46* D410* P61* R7*F414* P56* D510* S62*~{R2}

V [1]

P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-* R10* B1*B3* S42* D40* S50* P40* D30* S40* S41* R2* P30* P24* S30* D36*~{D310}

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30* S52* P46* D410*P56* S61* P31

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* S41* R2* D38* P34

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S41* R2* P41* P44

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S41* R2* P41* P54* S52* P46* D410

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S41* S52* P46* D410* P44* R5* P51

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S41* R2* P44* D36

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30* P41* P46* S51*~{D410* R5}

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* P34* S52* P46* D410* S51* P61* R7*F414* P56* D510* S62

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* R2* P34* P46* D36* S51*~{D410* R5}

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* R2* P46* P44* D36* S51*~{D410* R5}

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* R2* P34* S52* P46* D410* D36* P56*S61

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* B1* B3* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30* P46* D410* R5*S51* P31

Concept FOR CLASS without compound ABX_2 :

[4]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* S42* D40* S50* P40* B2* R3*~{R2}*~{P54* S52* P46* D410* P61* R7* F414*P56* D510* S62}

V [4]

P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10*S42* D40* S50* D30* S40*~{D310* B1* B3* P40}*~{P34}*~{B1* B3* P40* P30}*~{B1*B3* P40* R2* P30* P24* S30}*~{D310* P40* R2* P44* P31* B2* R3}*~{D310* P40*R2* P54* S52* P46* D410* P31* B2* R3}

V [3]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* S42* D40* S50* P40* D30* S40* R2* P30* P24* S30* B2* R3

V [2]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* S42* D40* S50* S52* P46* D410* P61* R7* F414* P56* D510* S62* B2*~{P40*D30* S40* P34}*~{P40* P54* R3}*~{P44* R5}

V [1]

D310* P36* S12* S22* P26* S32* F40* P50* D50* F50* S60* P60* D60* S70* B2-*R10* S42* D40* S50* P40* D30* S40* P34* S52* P46* D410* P61* R7* F414* P56*D510* S62* B2* R3

Feature set IV

Concept FOR CLASS chalcopyrite :

[38]
S* R10* P* B2-*~{B1* B3}*~{I13}*~{TM3}
V [17]
S* R10* P* B2-* B1* B3* I46* E3*~{TD6* TM5* H5* C5* I28* E4* S5* I17* I38}*~{I13* TM3* I28* I38* TM2* I110* TD1* I11* E2* C2* I45* TD5* S3* R9* I29* H1*S8* I35* C6* H2}*~{I13* TM3* I28* I38* TM2* I110* TD1* I11* E2* C2* I45* TD5*S3* R9* I29* H1* S8* I35* C6* H2* C9* E1* I48* I39* I210}*~{TM3* TD6* TM5* H5*C5* I28* E4* S5* I17* I38* C6* I27* I36* S2* R3* I19* I42* TD3* S6* H7* I26*I47* E8* TD9* H8* D* TM7}*~{TD6* TM5* H5* C5* I28* E4* S5* I17* I38* TM2*I110* TD1* C6* I36* S2* R3* I26* I47* E8* TD9* H8* D* TM7* I43* H3}
V [16]
S* R10* P* B2-* B1* B3* E3* C3* R8* TD8*~{I27}*~{H5* I28* I17* I38* TM2* I110*C2* I45* TD5* S3* I29* H1* C6* I48* S2* R3* I26* I47* E8* TD9* H8* D* TM7* E5*TM6* S4}*~{C5* S5* TM2* TD1* I36* I43* H3}
V [10]
S* R10* P* B2-* I13* E3* C5* I28* E4* S5* I27* I36*~{TM3* TM2* I110* TD1* S2*TD9* I43* H3* C3* R2* H4* I410* I34}*~{B1* B3* TM3* TM2* I110* TD1* I11* S8*H2* C9* E1* I48* I39* I210* S2* TD9* I43* H3* C3* R2* H4* I410* I34}*~{TM3*C6* H2* C9* I48* R3* H3* TD8* TM1}
V [10]
S* R10* P* B2-* I13* TM3* I28* TD1*~{I46* E2* S8* I35* C6* H2} {B1* B3* I46*E3* I38* TM2* I110* I11* E2* C2* I45* TD5* S3* R9* I29* H1* S8* I35* C6* H2}*~{E3* TM2* I110}*~{B1* B3* I46* E3* I38* TM2* I110* I11* E2* C2* I45* TD5*S3* R9* I29* H1* S8* I35* C6* H2* C9* E1* I48* I39* I210}*~{E3* C5* E4* S5*TM2* I110* I27* I36* S2* TD9* I43* H3* C3* R2* H4* I410* I34}*~{B1* B3* E3*C5* E4* S5* TM2* I110* I11* S8* H2* C9* E1* I48* I39* I210* I27* I36* S2* TD9*I43* H3* C3* R2* H4* I410* I34}*~{B1* B3* E3* C5* E4* S5* TM2* I11* S8* C6*H2* C9* E1* I48* I39* I210* I27* I36* R3* I19* I42* TD3* S6* H7* H3* TD8* TM1}*~{I46* E3* C5* S5* TM2* I110* E2* TD5* S8* I35* C6* H2* E1* I39* I36* I19*I47* I43* H3* R8* B2* S7* I25* C1}
V [9]
S* R10* P* B2-* B1* B3* I46* I35*~{I13* TM3* E3* I28* I38* TM2* I110* TD1*I11* E2* C2* I45* TD5* S3* R9* I29* H1* S8* C6* H2}*~{I13* TM3* E3* I28* I38*TM2* I110* TD1* I11* E2* C2* I45* TD5* S3* R9* I29* H1* S8* C6* H2* C9* E1*I48* I39* I210}*~{I13* TM3* I28* TD1* E2* R9* H1* S8* C6* H2* C9* TM1}*~{I13*TM3* TD6* TM5* H5* C5* I28* E4* S5* I17* I38* TD1* E2* R9* H1* S8* C6* H2* C9*I210* TM1* I49* I111* S12* B6* I310}*~{I13* TM3* I28* TD1* I11* E2* R9* H1*S8* C6* H2* C9* I210* TM1* I111* S12* B6* I310}
V [9]
S* R10* P* B2-* B1* B3* E3* H5* I28* I17* I38* I48* I27* C3* R8* TD8* E5* TM6*S4
V [9]
S* R10* P* B2-* B1* B3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17* I38* I27*~{TM3* C6* I36* S2* R3* I19* I42* TD3* S6* H7* I26* I47* E8* TD9* H8* D* TM7}*~{TM2* H1* H2* C9* I210* R8* I34* TM1* S7* I49* I111* S12* B6* I310* C7* I12*TD2}
V [7]
S* R10* P* B2-* B1* B3* E3* TM2* H2* I27* R8* I34* S7* I49* C7* I12* TD2*~{I110* E1}*~{I46* TD6* TM5* H5* C5* I28* E4* S5* I17* I38* H1* C9* I210* TM1*I111* S12* B6* I310}*~{I11* E2* H1* C9* I210* S2* C3* TD8* TM1*

I111* S12* B6*I310* R4}*~{C5* I28* S5* I110* TD1* I11* E2* I210* I36* S2* I43* H3* C3* TD8*I310* R4}*~{I11* H1* C9* E1* I210* I410* TM1* I111* S12* B6* I310* TD4}*~{TD1* I11* H1* S8* C9* E1* I48* I39* I210* TM1* I111* S12* B6* I310}*~{TD1*I11* I29* H1* C9* E1* I39* I210* I47* TM1* I111* S12* B6* I310* S10}*~{TM3*C5* I11* C9* E1* I210* I36* I19* I42* TD3* S6* H7* I410* I310* TD4}*~{TM3* C5*TD1* I11* S8* C9* E1* I48* I39* I210* I36* I19* I42* TD3* S6* H7}

V [7]

S* R10* P* B2-* I13* TM3* E3* C5* I28* E4* S5* I48* I27* I36* H3*~{B1* B3*TM2* I110* TD1* I11* S8* H2* C9* E1* I39* I210* S2* TD9* I43* C3* R2* H4*I410* I34}*~{C6* H2* C9* R3* TD8* TM1}

V [7]

S* R10* P* B2-* B1* B3* E3* S2* C3* I34*~{I13* TM3* C5* I28* E4* S5* TM2*I110* TD1* I11* S8* H2* C9* E1* I48* I39* I210* I27* I36* TD9* I43* H3* R2*H4* I410}*~{I11* E2* H2* I210* I27* R8* TD8* S7* I49* I310* R4}*~{I13* TM3*E4* I38* TM2* I110* I11* E2* C2* I45* TD5* S3* I29* H1* H2* I210* I27* TD9*TD8* R2* H4* I410* I310* R4}*~{I13* TM3* C5* E4* TM2* TD1* I11* S8* H2* C9*E1* I48* I39* I210* I27* I36* I19* I42* TD3* S6* H7* TD9* R2* H4* I410}*~{I13* TM3* C5* I28* E4* S5* TM2* I110* TD1* I11* H2* C9* E1* I210* I27* I36*TD9* I43* H3* R8* R2* H4* I410* S7* I310* TD4}*~{I13* TM3* C5* E4* TM2* I11*H2* C9* E1* I210* I27* I36* I19* I42* TD3* S6* H7* TD9* R8* R2* H4* I410* S7*I310* TD4}

V [6]

S* R10* P* B2-* I13* TM3* I28* I17* I27* S2* TD9* C3* R2* H4* I410* I34*~{B1*B3* I46* TD6* TM5* H5* C5* E4* S5* I38* H1* C9* I210* TM1* I49* I111* S12* B6*I310}*~{B1* B3* H5* E4* I38* H1* C9* I48* I210* R8* TD8* E5* TM6* S4* TM1*I49* I111* S12* B6* I310}

V [6]

S* R10* P* B2-* I13* TM3* I28* I27* S2* TD9* C3* R2* H4* I410* I34*~{E3* C5*E4* S5* TM2* I110* TD1* I36* I43* H3}*~{B1* B3* I46* TD6* TM5* H5* C5* E4* S5*I17* I38* H1* C9* I210* TM1* I49* I111* S12* B6* I310}*~{B1* B3* H5* E4* I17*I38* H1* C9* I48* I210* R8* TD8* E5* TM6* S4* TM1* I49* I111* S12* B6* I310}

V [6]

S* R10* P* B2-* B1* B3* I13* TM3* E3* E4* I27* S2* TD9* C3* R2* H4* I410* I34*~{C5* I28* S5* TM2* I110* TD1* I11* S8* H2* C9* E1* I48* I39* I210* I36* I43*H3}*~{I38* TM2* I110* I11* E2* C2* I45* TD5* S3* I29* H1* H2* I210* TD8* I310*R4}*~{C5* TM2* TD1* I11* S8* H2* C9* E1* I48* I39* I210* I36* I19* I42* TD3*S6* H7}*~{C5* I28* S5* TM2* I110* TD1* I11* H2* C9* E1* I210* I36* I43* H3*R8* S7* I310* TD4}*~{C5* TM2* I11* H2* C9* E1* I210* I36* I19* I42* TD3* S6*H7* R8* S7* I310* TD4}

V [6]

S* R10* P* B2-* I13* I28* E4* S5* C6* I48* I36* R3* H3* TD8* TM1*~{B1* B3*TM3* E3* C5* TM2* TD1* I11* S8* H2* C9* E1* I39* I210* I27* I19* I42* TD3* S6*H7}*~{B1* B3* E3* I38* TM2* I110* TD1* I11* C2* I45* TD5* S3* I29* H1* E1*S10* C10* I44}*~{B1* B3* TM2* TD1* I11* I29* H1* C9* E1* I39* I210* I47* I49*I111* S12* B6* I310* S10}*~{B1* B3* TM2* I11* E2* H1* H2* C9* I210* S2* C3*I49* I111* S12* B6* I310* R4}*~{B1* B3* TM2* I11* H1* H2* C9* E1* I210* R8*I410* S7* I49* I111* S12* B6* I310* TD4}*~{B1* B3* H5* I17* I38* H1* C9* I210*C3* R8* E5* TM6* S4* I49* I111* S12* B6* I310}*~{B1* B3* I46* TD6* TM5* H5*C5* I17* I38* H1* C9* I210* I49* I111* S12* B6* I310}*~{B1* B3* TM3* E3* C5*TM2* I11* H2* C9* E1* I210* I27* I19* I42* TD3* S6* H7* R8* I410* S7* I310*TD4}*~{B1* B3* E3* I38* TM2* I110* TD1* I11* C2* I45* TD5* S3* I29* H1* S8*H2* C9* E1* I39* I210}*~{B1* B3* E3* C5* TM2*

I110* TD1* I11* S8* H2* C9* E1*I39* I210* I43}*~{B1* B3* TM2* TD1* I11* H1* S8* H2* C9* E1* I39* I210* I49*I111* S12* B6* I310}

V [6]

S* R10* P* B2-* I13* I28* E4* S5* C6* I48* I36* R3* H3* TD8* TM1*~{TM3* E3*C5* H2* C9* I27}*~{B1* B3* TM3* E3* C5* TM2* TD1* I11* S8* H2* C9* E1* I39*I210* I27* I19* I42* TD3* S6* H7}*~{B1* B3* E3* I38* TM2* I110* TD1* I11* C2*I45* TD5* S3* I29* H1* E1* S10* C10* I44}*~{B1* B3* TM2* TD1* I11* I29* H1*C9* E1* I39* I210* I47* I49* I111* S12* B6* I310* S10}*~{B1* B3* TM2* I11* E2*H1* H2* C9* I210* S2* C3* I49* I111* S12* B6* I310* R4}*~{B1* B3* TM2* I11*H1* H2* C9* E1* I210* R8* I410* S7* I49* I111* S12* B6* I310* TD4}*~{B1* B3*H5* I17* I38* H1* C9* I210* C3* R8* E5* TM6* S4* I49* I111* S12* B6* I310}*~{B1* B3* I46* TD6* TM5* H5* C5* I17* I38* H1* C9* I210* I49* I111* S12* B6*I310}*~{B1* B3* TM3* E3* C5* TM2* I11* H2* C9* E1* I210* I27* I19* I42* TD3*S6* H7* R8* I410* S7* I310* TD4}*~{B1* B3* E3* I38* TM2* I110* TD1* I11* C2*I45* TD5* S3* I29* H1* S8* H2* C9* E1* I39* I210}*~{B1* B3* E3* C5* TM2* I110*TD1* I11* S8* H2* C9* E1* I39* I210* I43}*~{B1* B3* TM2* TD1* I11* H1* S8* H2*C9* E1* I39* I210* I49* I111* S12* B6* I310}

V [6]

S* R10* P* B2-* B1* B3* I38* H2* I49*~{TM2* I110* C2* I45* TD5* S3* I29* H1}*~{C5* I28* E4* S5* H1* C9* I210* TM1* I111* S12* B6* I310}*~{I13* TM3* I46*I28* TD1* I11* E2* R9* I29* H1* S8* I35* C6* C9* E1* I210* TM1* I111* S12* B6*I310* S10* C10* I44}*~{I17* TM2* I11* E2* H1* C6* C9* I210* S2* R3* I26* I47*E8* TD9* H8* D* TM7* C3* TD8* TM1* I111* S12* B6* I310* R4}*~{I17* TM2* I11*H1* C6* C9* E1* I210* S2* R3* I26* I47* E8* TD9* H8* D* TM7* R8* I410* TM1*S7* I111* S12* B6* I310* TD4}

V [6]

S* R10* P* B2-* B1* B3* E3* I35* S2* I47* D* TM7* I25* R4* C4* I18* E7* TD10*H6*~{TM2* I110}

V [6]

S* R10* P* B2-* B1* B3* E3* I28* S5* TD1* I48* I36* H3*~{I13* TM3* C5* E4*TM2* I110* I11* S8* H2* C9* E1* I39* I210* I27* S2* TD9* I43* C3* R2* H4*I410* I34}*~{I13* TM3* C5* E4* TM2* I11* S8* C6* H2* C9* E1* I39* I210* I27*R3* I19* I42* TD3* S6* H7* TD8* TM1}*~{I13* E4* I38* TM2* I110* I11* C2* I45*TD5* S3* I29* H1* C6* E1* R3* TD8* TM1* S10* C10* I44}*~{I13* E4* I38* TM2*I110* I11* C2* I45* TD5* S3* I29* H1* S8* C6* H2* C9* E1* I39* I210* R3* TD8*TM1}*~{I13* C5* E4* TM2* I110* I11* S8* C6* H2* C9* E1* I39* I210* R3* I43*TD8* TM1}*~{C5* TM2* I110* I11* S8* I35* H2* C9* E1* I39* I210* S2* I47* D*TM7* I43* I25* R4* C4* I18* E7* TD10* H6}*~{C5* TM2* I110* I11* S8* H2* C9*E1* I39* I210* I27* I43* R8* I34* S7* I49* C7* I12* TD2}

V [5]

S* R10* P* B2-* B1* B3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17* I38* I35

V [4]

S* R10* P* B2-* B1* B3* TM2* H2* C3* I49*~{I11* C9* I210* I310}*~{I28* I36}*~{E8* TD9}*~{I13* TM3* E4* I11* H1* C9* E1* I210* I27* S2* TD9* R8* R2* H4*I410* I34* TM1* S7* I111* S12* B6* I310* TD4}*~{I13* TM3* E4* I11* H1* C9*I210* I27* S2* TD9* R2* H4* I410* I34* TM1* I111* S12* B6* I310}

V [2]

S* R10* P* B2-* B1* B3* E3* C5* I28* S5* TM2* I110* TD1* I35* I36* S2* I47* D*TM7* I43* H3* I25* R4* C4* I18* E7* TD10* H6*~{I11* S8* H2* C9* E1* I48* I39*I210}*~{I38* I11* I29* H1* E1* TM1* S10* C10* I44}*~{I11* I29* H1* C9* E1*I39* S10}

V [1]

S* R10* P* B2-* B1* B3* TM3* E3* C5* TM2* I11* E2* H2* I210* I27* I36*

S2*I19* I42* TD3* S6* H7* C3* R8* TD8* I34* S7* I49* I310* C7* I12* TD2* R4
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* E3* H5* I28* E4* I17* I38* TM2* I110*
C2*I45* TD5* S3* I29* H1* I48* I27* S2* TD9* C3* R8* TD8* E5* TM6* S4* R2*
H4*I410* I34
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* E3* H5* C5* I28* E4* S5* I17* I38*
TM2*I110* TD1* I48* I27* I36* S2* TD9* I43* H3* C3* R8* TD8* E5* TM6* S4*
R2* H4*I410* I34
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* E3* H5* C5* I28* E4* I17* I38* I48*
I27*I36* S2* I19* I42* TD3* S6* H7* TD9* C3* R8* TD8* E5* TM6* S4* R2* H4*
I410*I34
V [1]
S* R10* P* B2-* B1* B3* I13* E3* H5* C5* I28* E4* S5* I17* I38* TM2*
I110*TD1* C6* I48* I36* R3* I43* H3* C3* R8* TD8* E5* TM6* S4* TM1
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* E3* H5* C5* I28* E4* S5* I17* I38* C6*
I48*I27* I36* R3* I19* I42* TD3* S6* H7* H3* C3* R8* TD8* E5* TM6* S4* TM1
V [1]
S* R10* P* B2-* B1* B3* E3* H5* C5* I28* S5* I17* I38* TM2* I110* TD1*
H2*I48* I27* I36* I43* H3* C3* R8* TD8* E5* TM6* S4* I34* S7* I49* C7* I12*
TD2
V [1]
S* R10* P* B2-* B1* B3* TM3* E3* H5* C5* I28* I17* I38* TM2* H2* I48*
I27*I36* I19* I42* TD3* S6* H7* C3* R8* TD8* E5* TM6* S4* I34* S7* I49* C7*
I12*TD2
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* I46* E3* H5* I28* I17* I38* TM2* I110*
TD1*E2* C2* I45* TD5* S3* R9* I29* H1* S8* I35* C6* H2* I48* C3* R8* TD8*
E5* TM6*S4
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* I46* E3* H5* C5* I28* S5* I17* I38*
TM2*I110* TD1* E2* R9* S8* I35* C6* H2* I48* I36* I43* H3* C3* R8* TD8* E5*
TM6*S4
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* I46* E3* H5* C5* I28* I17* I38* TD1* E2*
R9*S8* I35* C6* H2* I48* I27* I36* I19* I42* TD3* S6* H7* C3* R8* TD8* E5*
TM6*S4
V [1]
S* R10* P* B2-* B1* B3* E3* H5* I28* I17* I38* TM2* I110* C2* I45* TD5*
S3*I29* H1* I35* I48* S2* I47* D* TM7* C3* R8* TD8* E5* TM6* S4* I25* R4*
C4*I18* E7* TD10* H6
V [1]
S* R10* P* B2-* B1* B3* TM3* E3* H5* C5* I28* I17* I38* I35* I48* I27*
I36*S2* I19* I42* TD3* S6* H7* I47* D* TM7* C3* R8* TD8* E5* TM6* S4* I25*
R4* C4*I18* E7* TD10* H6
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5*
I17*I38* TM2* I110* C2* I45* TD5* S3* I29* H1* I27* S2* TD9* C3* R2* H4*
I410*I34
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5*
I17*I38* TM2* I110* TD1* I27* I36* S2* TD9* I43* H3* C3* R2* H4* I410* I34

V [1]
S* R10* P* B2-* B1* B3* I13* TM3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17*I38* I27* I36* S2* I19* I42* TD3* S6* H7* TD9* C3* R2* H4* I410* I34
V [1]
S* R10* P* B2-* B1* B3* I13* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17* I38*TM2* I110* TD1* C6* I48* I36* R3* I43* H3* TD8* TM1
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17*I38* C6* I48* I27* I36* R3* I19* I42* TD3* S6* H7* H3* TD8* TM1
V [1]
S* R10* P* B2-* B1* B3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17* I38* TM2*I110* TD1* H2* I27* I36* I43* H3* R8* I34* S7* I49* C7* I12* TD2
V [1]
S* R10* P* B2-* B1* B3* TM3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17* I38*TM2* H2* I27* I36* I19* I42* TD3* S6* H7* R8* I34* S7* I49* C7* I12* TD2
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17*I38* TM2* I110* TD1* E2* R9* S8* I35* C6* H2* I36* I43* H3
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17*I38* TD1* E2* R9* S8* I35* C6* H2* I27* I36* I19* I42* TD3* S6* H7
V [1]
S* R10* P* B2-* B1* B3* I46* TD6* TM5* H5* C5* I28* E4* S5* I17* I38* H1* I35*C9* I210* S2* I47* D* TM7* TM1* I25* I49* I111* S12* B6* I310* R4* C4* I18* E7* TD10* H6
V [1]
S* R10* P* B2-* B1* B3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17* I38* TM2*I110* C2* I45* TD5* S3* I29* H1* I35* S2* I47* D* TM7* I25* R4* C4* I18* E7*TD10* H6
V [1]
S* R10* P* B2-* B1* B3* TM3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17* I38*I35* I27* I36* S2* I19* I42* TD3* S6* H7* I47* D* TM7* I25* R4* C4* I18* E7*TD10* H6
V [1]
S* R10* P* B2-* I13* TM3* E3* E4* S5* I38* TM2* I110* E2* C2* I45* TD5* S3*I29* H1* I48* I39* I27* S2* I26* TD9* H3* C3* H4* I410* I34* B2* C1* R6* TD7
V [1]
S* R10* P* B2-* I13* TM3* E3* C5* I28* E4* S5* TM2* I110* TD1* E2* I48* I39*I27* I36* S2* I26* TD9* I43* H3* C3* H4* I410* I34* B2* C1* R6* TD7
V [1]
S* R10* P* B2-* I13* TM3* E3* C5* E4* S5* I110* E2* I48* I39* I27* I36* S2*I19* I42* TD3* S6* H7* I26* TD9* H3* C3* H4* I410* I34* B2* C1* R6* TD7
V [1]
S* R10* P* B2-* I13* TM3* E3* C5* I28* E4* S5* I110* E2* C6* I48* I39* I27*I36* I19* I42* TD3* S6* H7* I26* H3* TD8* TM1* B2* C1* R6* TD7
V [1]
S* R10* P* B2-* I13* TM3* I46* E3* C5* I28* S5* I110* TD1* E2* S8* I35* C6*H2* I48* I39* I27* I36* I19* I42* TD3* S6* H7* I26* H3* B2* C1* R6* TD7
V [1]
S* R10* P* B2-* I13* TM3* E3* C5* I28* E4* S5* TD5* C6* E1* I48* I39* I27*I36* I19* I42* TD3* S6* H7* I47* H3* R8* TD8* TM1* B2* S7* I25* C1
V [1]
S* R10* P* B2-* I13* TM3* E3* C5* I28* E4* S5* I110* TD1* C6* H2* C9*

I48*I27* I36* I19* I42* TD3* S6* H7* H3* TD8* TM1* B2* S10* I44* I37
V [1]
S* R10* P* B2-* B1* B3* E3* H5* I28* I17* I38* TM2* I110* C2* I45* TD5*
S3*I29* H1* H2* I48* I27* C3* R8* TD8* E5* TM6* S4* I34* S7* I49* C7* I12*
TD2
V [1]
S* R10* P* B2-* B1* B3* E3* H5* C5* I28* S5* I17* I38* TM2* I110* TD1*
I35*I48* I36* S2* I47* D* TM7* I43* H3* C3* R8* TD8* E5* TM6* S4* I25* R4*
C4*I18* E7* TD10* H6
V [1]
S* R10* P* B2-* B1* B3* I13* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17*
I38*TM2* I110* C2* I45* TD5* S3* I29* H1* C6* I48* I36* R3* H3* TD8* TM1
V [1]
S* R10* P* B2-* B1* B3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17* I38*
TM2*I110* C2* I45* TD5* S3* I29* H1* H2* I27* R8* I34* S7* I49* C7* I12* TD2

Concept FOR CLASS b-$NaFeO_2$:

[5]
S* R10* P* B2-* B1* B3* I210* I310*~{I49}*~{H2* E1* R8* S7* TD4}
V [3]
S* R10* P* B2-* I13* E4* I11* H1* H2* C9* I210* TM1* I111* S12* B6*
I310*~{B1* B3* I28* S5* TM2* TD1* S8* C6* E1* I48* I39* I36* R3* H3* TD8*
I49}*~{B1*B3* TM3* TM2* I27* S2* TD9* C3* R2* H4* I410* I34* I49}
V [3]
S* R10* P* B2-* I13* H1* H2* C9* TM1*~{E4* S5* C6* I48* R3* H3* TD8}*~{B1*
B3*TM3* I46* I28* TD1* E2* R9* S8* I35* C6}*~{B1* B3* TM3* I46* I28* TD1*
I11*E2* R9* S8* I35* C6* I210* I111* S12* B6* I310}*~{B1* B3* I28* E4* S5*
TM2*TD1* I11* S8* C6* E1* I48* I39* I210* I36* R3* H3* TD8* I49* I111* S12*
B6*I310}*~{B1* B3* TM3* E4* TM2* I11* I210* I27* S2* TD9* C3* R2* H4*
I410* I34*I49* I111* S12* B6* I310}*~{TM3* I46* E3* I28* I38* TM2* I110*
TD1* E2* C2*I45* TD5* S3* I29* S8* I35* C6* I27* B2* S10* I44* I37}
V [2]
S* R10* P* B2-* B1* B3* I28* TM2* H2* I36* C3* I49*~{TM3* E3* H5* C5*
I17*I38* I48* I27* I19* I42* TD3* S6* H7* R8* TD8* E5* TM6* S4* I34* S7* C7*
I12*TD2}*~{E3* H5* C5* S5* I17* I38* I110* TD1* I48* I27* I43* H3* R8* TD8*
E5*TM6* S4* I34* S7* C7* I12* TD2}
V [2]
S* R10* P* B2-* I13* TM3* E4* I27* S2* TD9* C3* R2* H4* I410* I34*~{B1*
B3*E3}*~{B1* B3* I46* TD6* TM5* H5* C5* I28* S5* I17* I38* H1* C9* I210*
TM1*I49* I111* S12* B6* I310}*~{B1* B3* H5* I28* I17* I38* H1* C9* I48*
I210* R8*TD8* E5* TM6* S4* TM1* I49* I111* S12* B6* I310}*~{B1* B3* TM2*
TD1* I11* H1*S8* H2* C9* E1* I48* I39* I210* TM1* I49* I111* S12* B6*
I310}*~{B1* B3* I38*TD1* I11* I29* H1* C9* E1* I210* TM1* I49* I111* S12*
B6* I310* S10* C10* I44}*~{B1* B3* TM2* I11* E2* H1* H2* C9* I210* TD8*
TM1* I49* I111* S12* B6* I310*R4}
V [2]
S* R10* P* B2-* B1* B3* TM2* I11* H2* C9* I210* C3* I49* I310*~{E2* H1*
S2*TD8* TM1* I111* S12* B6* R4}*~{TD1* H1* S8* E1* I48* I39* TM1* I111*
S12* B6}*~{E3* E2* H1* I27* S2* R8* TD8* I34* TM1* S7* I111* S12* B6* C7*
I12* TD2*R4}*~{I17* H1* E1* S2* R3* I26* I47* E8* TD9* D* TM7* R8* I410*
TM1* S7* I111*S12* B6* TD4* H6* I37}
V [2]
S* R10* P* B2-* B1* B3* TM2* I11* H1* H2* C9* E1* I210* R8* I410* TM1*

S7*I49* I111* S12* B6* I310* TD4*~{I17* S2* R3* I26* I47* TD9* D* TM7}*~{E3* I27*I34* C7* I12* TD2}*~{I35* S2* I47* D* TM7* I25* R4* C4* I18* E7* TD10* H6}*~{I13* TM3* I46* I28* TD1* E2* R9* S8* I35* C6}

V [2]

S* R10* P* B2-* B1* B3* I11* H1* H2* C9* I210* TD8* TM1* I49* I111* S12* B6*I310*~{TM2* E2* S2* C3* R4}*~{I13* I28* E4* S5* TM2* TD1* S8* C6* E1* I48*I39* I36* R3* H3}

V [1]

S* R10* P* B2-* B1* B3* I13* TM3* E3* E4* I38* TM2* I110* I11* E2* C2* I45*TD5* S3* I29* H1* H2* I210* I27* S2* TD9* C3* TD8* R2* H4* I410* I34* I310*R4

V [1]

S* R10* P* B2-* B1* B3* I13* I28* E4* S5* TM2* I11* E2* H1* C6* H2* C9* I48*I210* I36* S2* R3* H3* C3* TD8* TM1* I49* I111* S12* B6* I310* R4

V [1]

S* R10* P* B2-* B1* B3* E3* C5* I28* S5* TM2* I110* TD1* I11* E2* H2* I210*I27* I36* S2* I43* H3* C3* R8* TD8* I34* S7* I49* I310* C7* I12* TD2* R4

V [1]

S* R10* P* B2-* B1* B3* E3* I27* C3* R8* TD8*~{H5* I28* I17* I38* I48* E5*TM6* S4}*~{I13* TM3* I46* H5* C5* I28* I17* I38* TD1* E2* R9* S8* I35* C6* H2*I48* I36* I19* I42* TD3* S6* H7* E5* TM6* S4}*~{TM3* H5* C5* I28* I17* I38*TM2* H2* I48* I36* I19* I42* TD3* S6* H7* E5* TM6* S4* I34* S7* I49* C7* I12*TD2}*~{TM3* C5* TM2* I11* E2* H2* I210* I36* S2* I19* I42* TD3* S6* H7* I34*S7* I49* I310* C7* I12* TD2* R4}*~{TM3* H5* C5* I28* I17* I38* I35* I48* I36*S2* I19* I42* TD3* S6* H7* I47* D* TM7* E5* TM6* S4* I25* R4* C4* I18* E7*TD10* H6}*~{I13* TM3* H5* C5* I28* E4* I17* I38* I48* I36* S2* I19* I42* TD3*S6* H7* TD9* E5* TM6* S4* R2* H4* I410* I34}*~{I13* TM3* H5* C5* I28* E4* S5*I17* I38* C6* I48* I36* R3* I19* I42* TD3* S6* H7* H3* E5* TM6* S4* TM1}*~{I13* TM3* H5* C5* I28* E4* S5* I17* I38* TM2* I110* TD1* I48* I36* S2* TD9*I43* H3* E5* TM6* S4* R2* H4* I410* I34}*~{I13* TM3* H5* I28* E4* I17* I38*TM2* I110* C2* I45* TD5* S3* I29* H1* I48* S2* TD9* E5* TM6* S4* R2* H4* I410*I34}*~{TM2* I11* E2* H1* H2* C9* I210* S2* I34* TM1* S7* I49* I111* S12* B6*I310* C7* I12* TD2* R4}

V [1]

S* R10* P* B2-* B1* B3* E3* I11* E2* H2* I210* I27* S2* C3* R8* TD8* I34* S7*I49* I310* R4*~{TM3* C5* TM2* I36* I19* I42* TD3* S6* H7* C7* I12* TD2}*~{TM2* H1* C9* TM1* I111* S12* B6* C7* I12* TD2}

V [1]

S* R10* P* B2-* B1* B3* E3* C5* S5* TM2* TD1* I36* I43* H3* C3* R8* TD8*~{I13* TM3* I46* H5* I28* I17* I38* I110* E2* R9* S8* I35* C6* H2* I48* E5* TM6*S4}*~{H5* I28* I17* I38* I110* I35* I48* S2* I47* D* TM7* E5* TM6* S4* I25*R4* C4* I18* E7* TD10* H6}*~{H5* I28* I17* I38* I110* H2* I48* I27* E5* TM6*S4* I34* S7* I49* C7* I12* TD2}*~{I13* H5* I28* E4* I17* I38* I110* C6* I48*R3* E5* TM6* S4* TM1}*~{I13* TM3* H5* I28* E4* I17* I38* I110* I48* I27* S2*TD9* E5* TM6* S4* R2* H4* I410* I34}

V [1]

S* R10* P* B2-* B1* B3* I13* TM3* E4* TM2* I11* H1* H2* C9* E1* I210* I27* S2*TD9* C3* R8* R2* H4* I410* I34* TM1* S7* I49* I111* S12* B6* I310* TD4

V [1]

S* R10* P* B2-* B1* B3* I13* I28* E4* S5* TM2* I11* H1* C6* H2* C9* E1* I48*I210* I36* R3* H3* R8* TD8* I410* TM1* S7* I49* I111* S12* B6* I310* TD4

Concept FOR CLASS a-$NaFeO_2$:

[25]
S* R10* P* B2-* B1* B3*~{I46* I35}*~{H2* I49}*~{E3}*~{I210* I310}
V [23]
S* R10* P* B2-* B1* B3* I210* I49* I310*~{H1* C9* TM1* I111* S12* B6}*~{TM3*E3* C5* TM2* I11* E2* H2* I27* I36* S2* I19* I42* TD3* S6* H7* C3* R8* TD8*I34* S7* C7* I12* TD2* R4}*~{E3* C5* I28* S5* TM2* I110* TD1* I11* E2* H2*I27* I36* S2* I43* H3* C3* R8* TD8* I34* S7* C7* I12* TD2* R4}*~{TM3* E3* C5*TM2* I11* H2* C9* E1* I27* I36* I19* I42* TD3* S6* H7* R8* I410* I34* S7* C7*I12* TD2* TD4}
V [9]
S* R10* P* B2-* I13*~{I28* I36}*~{TM3}*~{H1* H2* C9* TM1}
V [8]
S* R10* P* B2-* B1* B3* TM2* I11* H2* C9* I210* I410* I49* I310*~{H1* E1* R8*TM1* S7* I111* S12* B6* TD4}*~{TM3* E3* C5* E1* I27* I36* I19* I42* TD3* S6*H7* R8* I34* S7* C7* I12* TD2* TD4}*~{I13* TM3* E4* TD1* H1* S8* E1* I48* I39*I27* S2* TD9* C3* R2* H4* I34* TM1* I111* S12* B6}
V [8]
S* R10* P* B2-* B1* B3* TM2* H2* I410* I49*~{I11* H1* C9* E1* I210* R8* TM1*S7* I111* S12* B6* I310* TD4}*~{TM3* E3* C5* I11* C9* E1* I210* I27* I36* I19*I42* TD3* S6* H7* R8* I34* S7* I310* C7* I12* TD2* TD4}*~{I13* I28* E4* S5*I11* H1* C6* C9* E1* I48* I210* I36* R3* H3* R8* TD8* TM1* S7* I111* S12* B6*I310* TD4}*~{I13* TM3* E4* I11* H1* C9* E1* I210* I27* S2* TD9* C3* R8* R2*H4* I34* TM1* S7* I111* S12* B6* I310* TD4}*~{I13* TM3* E4* TD1* I11* H1* S8*C9* E1* I48* I39* I210* I27* S2* TD9* C3* R2* H4* I34* TM1* I111* S12* B6*I310}
V [7]
S* R10* P* B2-* B1* B3* H2* E1* I210* R8* S7* I310* TD4*~{E3* I410}*~{I13*TM3* E3* C5* I28* E4* S5* TM2* I110* TD1* I11* C9* I27* I36* S2* TD9* I43* H3*C3* R2* H4* I410* I34}*~{I13* TM3* E3* C5* E4* TM2* I11* C9* I27* I36* S2*I19* I42* TD3* S6* H7* TD9* C3* R2* H4* I410* I34}*~{I13* I28* E4* S5* TM2*I11* H1* C6* C9* I48* I36* R3* H3* TD8* I410* TM1* I49* I111* S12* B6}*~{I13*TM3* E4* TM2* I11* H1* C9* I27* S2* TD9* C3* R2* H4* I410* I34* TM1* I49*I111* S12* B6}
V [5]
S* R10* P* B2-* I13* TM3* I28* H2* C9* TM1*~{E3* C5* E4* S5* C6* I48* I27*I36* R3* H3* TD8}*~{C6* TD8}*~{I46* E3* TD1* I27* S10* I44* I37}
V [5]
S* R10* P* B2-* B1* B3* E3* TM2* H2* E1* I27* R8* I34* S7* I49* C7* I12* TD2*~{I110}*~{TM3* I19* I42* TD3* S6* H7}
V [5]
S* R10* P* B2-* B1* B3* C5* I28* E4* S5* H1* C9* I210* TM1* I49* I111* S12*B6* I310*~{I46* TD6* TM5* H5* I17* I38* I35* S2* I47* D* TM7* I25* R4* C4*I18* E7* TD10* H6}*~{I13* TM3* I46* TD6* TM5* H5* I17* I38* I27* S2* TD9* C3*R2* H4* I410* I34}
V [4]
S* R10* P* B2-* B1* B3* I13* TM3* I46* I28* TD1* I11* E2* R9* H1* S8* I35* C6*H2* C9* E1* I210* TM1* I111* S12* B6* I310
V [4]
S* R10* P* B2-* B1* B3* TM2* TD1* I11* H2* C9* I39* I210* I49* I310*~{H1* S8*E1* I48* TM1* I111* S12* B6}*~{H1* S8* E1* I48* I47* TM1* I111* S12* B6}
V [4]
S* R10* P* B2-* B1* B3* H1* C9* I210* C3* R8* TD8* TM1* I49* I111* S12*

B6*I310*~{E3* TM2* I11* E2* H2* I27* S2* I34* S7* C7* I12* TD2* R4}
V [3]
S* R10* P* B2-* B1* B3* E3* TM2* I11* H2* C9* E1* I210* R8* I410* S7* I49*I310* TD4*~{TM3* C5* I27* I36* I19* I42* TD3* S6* H7* I34* C7* I12* TD2}
V [3]
S* R10* P* B2-* B1* B3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17* I38*~{I27}*~{I35}*~{I13* TM2* I110* C2* I45* TD5* S3* I29* H1* C6* I48* I36* R3* H3*TD8* TM1}*~{I13* TM2* I110* TD1* C6* I48* I36* R3* I43* H3* TD8* TM1}
V [2]
S* R10* P* B2-* B1* B3* TM2* H2* E8* TD9* C3* I49*~{I17* TD1* I11* H1* S8* C9*E1* I48* I39* I210* S2* R3* I26* I47* D* TM7* TM1* I111* S12* B6* I310* H6*I37}
V [2]
S* R10* P* B2-* B1* B3* I17* TM2* I11* H1* H2* C9* E1* I210* S2* R3* I26* I47*TD9* D* TM7* R8* I410* TM1* S7* I49* I111* S12* B6* I310* TD4
V [2]
S* R10* P* B2-* B1* B3* C5* I28* E4* S5* I38* H1* H2* C9* I210* TM1* I49*I111* S12* B6* I310
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* E4* TM2* I11* E2* H1* H2* C9* I210* I27* S2*TD9* C3* TD8* R2* H4* I410* I34* TM1* I49* I111* S12* B6* I310* R4
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* E4* TM2* I11* H1* H2* C9* I210* I27* S2*TD9* C3* R2* H4* I410* I34* TM1* I49* I111* S12* B6* I310*~{E1* R8* S7* TD4}*~{TD1* S8* E1* I48* I39}
V [1]
S* R10* P* B2-* B1* B3* I17* I38* TM2* I11* E2* H1* C6* H2* C9* I210* S2* R3*I26* I47* E8* TD9* H8* D* TM7* C3* TD8* TM1* I49* I111* S12* B6* I310* R4
V [1]
S* R10* P* B2-* B1* B3* E3* I38* TM2* I110* I11* C2* I45* TD5* S3* I29* H1*H2* C9* E1* I210* I27* R8* I410* I34* S7* I49* I310* C7* I12* TD2* TD4
V [1]
S* R10* P* B2-* B1* B3* E3* C5* I28* S5* TM2* I110* TD1* I11* H2* C9* E1*I210* I27* I36* I43* H3* R8* I410* I34* S7* I49* I310* C7* I12* TD2* TD4
V [1]
S* R10* P* B2-* B1* B3* E3* TM2* I11* H1* H2* C9* E1* I210* I27* R8* I410*I34* TM1* S7* I49* I111* S12* B6* I310* C7* I12* TD2* TD4
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* I46* I28* TM2* TD1* I11* E2* R9* H1* S8*I35* C6* H2* C9* E1* I210* R8* I410* TM1* S7* I49* I111* S12* B6* I310* TD4
V [1]
S* R10* P* B2-* B1* B3* TM2* I11* H1* I35* H2* C9* E1* I210* S2* I47* D* TM7*R8* I410* TM1* S7* I25* I49* I111* S12* B6* I310* R4* TD4* C4* I18* E7* TD10*H6
V [1]
S* R10* P* B2-* B1* B3* I17* TM2* I11* H1* H2* C9* E1* I210* S2* R3* I26* I47*E8* TD9* D* TM7* C3* R8* I410* TM1* S7* I49* I111* S12* B6* I310* TD4* H6*I37
V [1]
S* R10* P* B2-* B1* B3* I17* I38* TM2* I11* H1* C6* H2* C9* E1* I210* S2* R3*I26* I47* E8* TD9* H8* D* TM7* R8* I410* TM1* S7* I49* I111* S12* B6*

I310*TD4
V [1]
S* R10* P* B2-* B1* B3* E3* TM2* TD1* I11* H1* S8* H2* C9* E1* I48* I39* I210*I27* R8* I34* TM1* S7* I49* I111* S12* B6* I310* C7* I12* TD2
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* I46* I28* TM2* TD1* I11* E2* R9* H1* S8*I35* C6* H2* C9* E1* I48* I39* I210* TM1* I49* I111* S12* B6* I310
V [1]
S* R10* P* B2-* B1* B3* E3* TM2* TD1* I11* I29* H1* H2* C9* E1* I39* I210*I27* I47* R8* I34* TM1* S7* I49* I111* S12* B6* I310* C7* I12* TD2* S10
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* I46* I28* TM2* TD1* I11* E2* R9* I29* H1*S8* I35* C6* H2* C9* E1* I39* I210* I47* TM1* I49* I111* S12* B6* I310* S10
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* I46* I28* I38* TD1* I11* E2* R9* I29* H1*S8* I35* C6* H2* C9* E1* I210* TM1* I49* I111* S12* B6* I310* S10* C10* I44
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* H5* I28* E4* I17* I38* H1* C9* I48* I210*I27* S2* TD9* C3* R8* TD8* E5* TM6* S4* R2* H4* I410* I34* TM1* I49* I111*S12* B6* I310
V [1]
S* R10* P* B2-* B1* B3* I13* H5* I28* E4* S5* I17* I38* H1* C6* C9* I48* I210*I36* R3* H3* C3* R8* TD8* E5* TM6* S4* T..I1* I49* I111* S12* B6* I310
V [1]
S* R10* P* B2-* B1* B3* I13* I46* TD6* TM5* H5* C5* I28* E4* S5* I17* I38* H1*C6* C9* I48* I210* I36* R3* H3* TD8* TM1* I49* I111* S12* B6* I310
V [1]
S* R10* P* B2-* B1* B3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17* I38* TM2*H1* H2* C9* I210* I27* R8* I34* TM1* S7* I49* I111* S12* B6* I310* C7* I12*TD2
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* I46* TD6* TM5* H5* C5* I28* E4* S5* I17*I38* TD1* E2* R9* H1* S8* I35* C6* H2* C9* I210* TM1* I49* I111* S12* B6*I310
V [1]
S* R10* P* B2-* B1* B3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17* I38* TM2*I110* TD1* C6* I36* S2* R3* I26* I47* E8* TD9* H8* D* TM7* I43* H3
V [1]
S* R10* P* B2-* B1* B3* TM3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17* I38*C6* I27* I36* S2* R3* I19* I42* TD3* S6* H7* I26* I47* E8* TD9* H8* D* TM7

Concept FOR CLASS TISe :

[7]
S* R10* P* B2-* TM3*~{I110}*~{I13* I46* E3* I28* I38* TM2* I110* TD1* E2* C2*I45* TD5* S3* I29* H1* S8* I35* C6* H2* B2}*~{B1* B3* I13* I46* E3* H5* I28*I17* I38* TM2* I110* TD1* E2* C2* I45* TD5* S3* R9* I29* H1* S8* I35* C6* H2*I48* C3* R8* TD8* E5* TM6* S4}*~{B1* B3* I13* I46* E3* I28* I38* TM2* I110*TD1* I11* E2* C2* I45* TD5* S3* R9* I29* H1* S8* I35* C6* H2* C9* E1* I48*I39* I210}*~{B1* B3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17* I38* TM2*H2* I27* I36* I19* I42* TD3* S6* H7* R8* I34* S7* I49* C7* I12* TD2}*~{B1* B3*I13* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17* I38* TD1*

E2* R9* S8* I35*C6* H2* I27* I36* I19* I42* TD3* S6* H7}*~{B1* B3* I13* I46* E3* H5* C5* I28*I17* I38* TD1* E2* R9* S8* I35* C6* H2* I48* I27* I36* I19* I42* TD3* S6* H7*C3* R8* TD8* E5* TM6* S4}*~{B1* B3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5*I17* I38* C6* I27* I36* S2* R3* I19* I42* TD3* S6* H7* I26* I47* E8* TD9* H8* D*TM7}*~{B1* B3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17* I38* I35* I27*I36* S2* I19* I42* TD3* S6* H7* I47* D* TM7* I25* R4* C4* I18* E7* TD10* H6}*~{B1* B3* I13* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17* I38* I27* I36*S2* I19* I42* TD3* S6* H7* TD9* C3* R2* H4* I410* I34}*~{B1* B3* I13* I46* E3*TD6* TM5* H5* C5* I28* E4* S5* I17* I38* C6* I48* I27* I36* R3* I19* I42* TD3*S6* H7* H3* TD8* TM1}*~{B1* B3* E3* H5* C5* I28* I17* I38* TM2* H2* I48* I27*I36* I19* I42* TD3* S6* H7* C3* R8* TD8* E5* TM6* S4* I34* S7* I49* C7* I12*TD2}*~{B1* B3* E3* C5* TM2* I11* E2* H2* I210* I27* I36* S2* I19* I42* TD3*S6* H7* C3* R8* TD8* I34* S7* I49* I310* C7* I12* TD2* R4}*~{B1* B3* E3* H5*C5* I28* I17* I38* I35* I48* I27* I36* S2* I19* I42* TD3* S6* H7* I47* D* TM7*C3* R8* TD8* E5* TM6* S4* I25* R4* C4* I18* E7* TD10* H6}*~{B1* B3* I13* E3*H5* C5* I28* E4* I17* I38* I48* I27* I36* S2* I19* I42* TD3* S6* H7* TD9* C3*R8* TD8* E5* TM6* S4* R2* H4* I410* I34}*~{B1* B3* I13* E3* H5* C5* I28* E4*S5* I17* I38* C6* I48* I27* I36* R3* I19* I42* TD3* S6* H7* H3* C3* R8* TD8*E5* TM6* S4* TM1}*~{I13* E3* C5* I28* E4* S5* TD5* C6* E1* I48* I39* I27* I36*I19* I42* TD3* S6* H7* I47* H3* R8* TD8* TM1* B2* S7* I25* C1}*~{B1* B3* I13*E3* C5* I28* E4* S5* TM2* TD1* I11* S8* C6* H2* C9* E1* I48* I39* I210* I27*I36* R3* I19* I42* TD3* S6* H7* H3* TD8* TM1}*~{B1* B3* I13* I46* TD6* TM5*H5* C5* I28* E4* S5* I17* I38* TD1* E2* R9* H1* S8* I35* C6* H2* C9* I210*TM1* I49* I111* S12* B6* I310}*~{B1* B3* I13* E3* H5* I28* E4* I17* I38* TM2*I110* C2* I45* TD5* S3* I29* H1* I48* I27* S2* TD9* C3* R8* TD8* E5* TM6* S4*R2* H4* I410* I34}*~{B1* B3* I13* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17*I38* TM2* I110* C2* I45* TD5* S3* I29* H1* I27* S2* TD9* C3* R2* H4* I410*I34}*~{B1* B3* I13* E3* E4* I38* TM2* I110* I11* E2* C2* I45* TD5* S3* I29*H1* H2* I210* I27* S2* TD9* C3* TD8* R2* H4* I410* I34* I310* R4}*~{B1* B3*I13* I46* TD6* TM5* H5* C5* I28* E4* S5* I17* I38* H1* C9* I210* I27* S2* TD9*C3* R2* H4* I410* I34* TM1* I49* I111* S12* B6* I310}*~{B1* B3* I13* H5* I28*E4* I17* I38* H1* C9* I48* I210* I27* S2* TD9* C3* R8* TD8* E5* TM6* S4* R2*H4* I410* I34* TM1* I49* I111* S12* B6* I310}*~{B1* B3* I13* I46* I28* I38*TD1* I11* E2* R9* I29* H1* S8* I35* C6* H2* C9* E1* I210* TM1* I49* I111* S12*B6* I310* S10* C10* I44}*~{B1* B3* I13* E4* TM2* I11* H1* H2* C9* E1* I210*I27* S2* TD9* C3* R8* R2* H4* I410* I34* TM1* S7* I49* I111* S12* B6* I310*TD4}*~{I13* E3* E4* S5* I38* TM2* I110* E2* C2* I45* TD5* S3* I29* H1* I48*I39* I27* S2* I26* TD9* H3* C3* H4* I410* I34* B2* C1* R6* TD7}*~{B1* B3* I13*E4* TM2* TD1* I11* H1* S8* H2* C9* E1* I48* I39* I210* I27* S2* TD9* C3* R2*H4* I410* I34* TM1* I49* I111* S12* B6* I310}*~{B1* B3* I13* E4* I38* TD1*I11* I29* H1* C9* E1* I210* I27* S2* TD9* C3* R2* H4* I410* I34* TM1* I49*I111* S12* B6* I310* S10* C10* I44}*~{B1* B3* I13* E4* TM2* I11* E2* H1* H2*C9* I210* I27* S2* TD9* C3* TD8* R2* H4* I410* I34* TM1* I49* I111* S12* B6*I310* R4}*~{B1* B3* I13* I46* I28* TM2* TD1* I11* E2* R9* H1* S8* I35* C6* H2*C9* E1* I210* R8* I410* TM1* S7* I49* I111* S12* B6* I310* TD4}*~{B1* B3* I13*I46* I28* TM2* TD1* I11* E2* R9* H1* S8* I35* C6* H2* C9* E1* I48* I39* I210*TM1* I49* I111* S12* B6* I310}*~{B1* B3* I13* I46* I28* TM2* TD1* I11* E2* R9*I29* H1* S8* I35* C6* H2* C9* E1* I39* I210* I47* TM1* I49* I111* S12* B6*I310* S10}*~{B1* B3* I13* I46* I28* TM2* TD1* I11* E2* R9* H1* S8* I35* C6*H2* C9* I210* S2* C3* TD8* TM1* I49* I111* S12* B6* I310* R4}*~{B1* B3* I13*I46* E3* I28* I38* TM2* I110* TD1* I11* E2* C2* I45* TD5* S3* R9* I29* H1* S8*I35* C6* H2* C9* E1* I39* I47* S10}*~{B1* B3* I13* I46* E3* I28* I38* TM2*I110* TD1* I11* E2*

C2* I45* TD5* S3* R9* I29* H1* S8* I35* C6* H2* E1* TM1*S10* C10*
I44}*~{I13* I46* E3* I28* S5* I38* TM2* I110* TD1* E2* C2* I45* TD5*S3* I29*
H1* S8* I35* C6* H2* I48* I39* I26* H3* B2* C1* R6* TD7}*~{I13* I46*E3* I28*
I38* TM2* I110* TD1* E2* C2* I45* TD5* S3* I29* H1* S8* I35* C6* H2*E1* I39*
I19* I47* H3* R8* B2* S7* I25* C1}

V [6]

S* R10* P* B2-* B1* B3* E3*~{I46}*~{I28* S5* TD1* H3}*~{I13* TM3* E4* I27*
S2*TD9* C3* R2* H4* I410* I34}*~{I35* S2* I47* D* TM7* I25* R4* C4* I18*
E7*TD10* H6}*~{TM2* H2* E1* I27* R8* I34* S7* I49* C7* I12* TD2}*~{TM2*
I11* H2*C9* E1* I210* R8* I410* S7* I49* I310* TD4}*~{C3}*~{TM2* I11* H1*
H2* C9* E1*I210* I27* R8* I410* I34* TM1* S7* I49* I111* S12* B6* I310* C7*
I12* TD2*TD4}*~{TM2* TD1* I11* H1* S8* H2* C9* E1* I48* I39* I210* I27* R8*
I34* TM1*S7* I49* I111* S12* B6* I310* C7* I12* TD2}*~{TM2* TD1* I11* I29*
H1* H2* C9*E1* I39* I210* I27* I47* R8* I34* TM1* S7* I49* I111* S12* B6*
I310* C7* I12*TD2* S10}*~{I38* TM2* I110* I11* C2* I45* TD5* S3* I29* H1*
H2* C9* E1* I210*I27* R8* I410* I34* S7* I49* I310* C7* I12* TD2* TD4}*~{C5*
I28* S5* TM2*I110* TD1* I11* H2* C9* E1* I210* I27* I36* I43* H3* R8* I410*
I34* S7* I49*I310* C7* I12* TD2* TD4}*~{C5* I28* S5* I17* I38* TM2* I110*
TD1* I11* C6* H2*C9* E1* I210* I36* S2* R3* I26* I47* E8* TD9* H8* D* TM7*
I43* H3* R8* I410*S7* I310* TD4}

V [5]

S* R10* P* B2-* I13* TM3*~{I28}*~{E3* C5* I28* E4* S5* I48* I27* I36*
H3}*~{I27}*~{B1* B3* E3* E4* I27* S2* TD9* C3* R2* H4* I410* I34}*~{B1* B3*
I46* E3*TD6* TM5* H5* C5* I28* E4* S5* I17* I38* TD1* E2* R9* S8* I35* C6*
H2* I27*I36* I19* I42* TD3* S6* H7}*~{B1* B3* I46* E3* H5* C5* I28* I17*
I38* TD1* E2*R9* S8* I35* C6* H2* I48* I27* I36* I19* I42* TD3* S6* H7* C3*
R8* TD8* E5*TM6* S4}*~{E3* C5* I28* E4* S5* TM2* I110* TD1* E2* I48* I39*
I27* I36* S2*I26* TD9* I43* H3* C3* H4* I410* I34* B2* C1* R6* TD7}*~{E3*
C5* I28* E4* S5*I110* E2* C6* I48* I39* I27* I36* I19* I42* TD3* S6* H7* I26*
H3* TD8* TM1*B2* C1* R6* TD7}*~{E3* C5* I28* E4* S5* TD5* C6* E1* I48* I39*
I27* I36* I19*I42* TD3* S6* H7* I47* H3* R8* TD8* TM1* B2* S7* I25*
C1}*~{E3* C5* I28* E4*S5* I110* TD1* C6* H2* C9* I48* I27* I36* I19* I42*
TD3* S6* H7* H3* TD8* TM1*B2* S10* I44* I37}*~{B1* B3* E3* E4* I38* TM2*
I110* I11* E2* C2* I45* TD5*S3* I29* H1* H2* I210* I27* S2* TD9* C3* TD8*
R2* H4* I410* I34* I310* R4}*~{E3* E4* S5* I38* TM2* I110* E2* C2* I45* TD5*
S3* I29* H1* I48* I39* I27*S2* I26* TD9* H3* C3* H4* I410* I34* B2* C1* R6*
TD7}*~{E3* C5* E4* S5* I110*E2* I48* I39* I27* I36* S2* I19* I42* TD3* S6*
H7* I26* TD9* H3* C3* H4* I410*I34* B2* C1* R6* TD7}*~{I46* E3* C5* I28*
S5* I110* TD1* E2* S8* I35* C6* H2*I48* I39* I27* I36* I19* I42* TD3* S6* H7*
I26* H3* B2* C1* R6* TD7}*~{I46*E3* I28* TD1* H2* C9* I27* TM1* S10* I44*
I37}

V [4]

S* R10* P* B2-* B1* B3* E3* H2* E1* I210* R8* I410* S7* I310* TD4*~{TM2*
I11*H1* C9* I27* I34* TM1* I49* I111* S12* B6* C7* I12* TD2}*~{I38* TM2*
I110*I11* C2* I45* TD5* S3* I29* H1* C9* I27* I34* I49* C7* I12* TD2}*~{C5*
I28*S5* TM2* I110* TD1* I11* C9* I27* I36* I43* H3* I34* I49* C7* I12*
TD2}*~{C5*I28* S5* I17* I38* TM2* I110* TD1* I11* C6* C9* I36* S2* R3* I26*
I47* E8*TD9* H8* D* TM7* I43* H3}

V [3]

S* R10* P* B2-* I13* TM3* I27* S2* TD9* C3* R2* H4* I410*
I34*~{I28}*~{E4}*~{B1* B3* E4* TM2* I11* H1* H2* C9* E1* I210* R8* TM1*
S7* I49* I111* S12*B6* I310* TD4}*~{B1* B3* E4* TM2* I11* H1* H2* C9* I210*
TM1* I49* I111* S12*B6* I310}

V [2]

S* R10* P* B2-* I13* TM3* E3* I28* TM2* I110* TD1*~{I46* E2* S8* I35* C6* H2*B2}*~{B1* B3* I46* H5* I17* I38* E2* C2* I45* TD5* S3* R9* I29* H1* S8* I35*C6* H2* I48* C3* R8* TD8* E5* TM6* S4}*~{B1* B3* I46* I38* I11* E2* C2* I45*TD5* S3* R9* I29* H1* S8* I35* C6* H2* C9* E1* I48* I39* I210}*~{B1* B3* I46*TD6* TM5* H5* C5* E4* S5* I17* I38* E2* R9* S8* I35* C6* H2* I36* I43* H3}*~{B1* B3* I46* H5* C5* S5* I17* I38* E2* R9* S8* I35* C6* H2* I48* I36* I43*H3* C3* R8* TD8* E5* TM6* S4}*~{B1* B3* I46* TD6* TM5* H5* C5* E4* S5* I17*I38* I27* I36* S2* TD9* I43* H3* C3* R2* H4* I410* I34}*~{B1* B3* C5* E4* S5*I11* S8* H2* C9* E1* I48* I39* I210* I27* I36* S2* TD9* I43* H3* C3* R2* H4*I410* I34}*~{B1* B3* H5* C5* E4* S5* I17* I38* I48* I27* I36* S2* TD9* I43*H3* C3* R8* TD8* E5* TM6* S4* R2* H4* I410* I34}*~{C5* E4* S5* E2* I48* I39*I27* I36* S2* I26* TD9* I43* H3* C3* H4* I410* I34* B2* C1* R6* TD7}*~{B1* B3*I46* I38* I11* E2* C2* I45* TD5* S3* R9* I29* H1* S8* I35* C6* H2* C9* E1*I39* I47* S10}*~{B1* B3* I46* I38* I11* E2* C2* I45* TD5* S3* R9* I29* H1* S8*I35* C6* H2* E1* TM1* S10* C10* I44}*~{I46* I38* E2* C2* I45* TD5* S3* I29*H1* S8* I35* C6* H2* E1* I39* I19* I47* H3* R8* B2* S7* I25* C1}

V [2]

S* R10* P* B2-* B1* B3* TM3* E3* TM2* H2* E1* I27* I19* I42* TD3* S6* H7* R8*I34* S7* I49* C7* I12* TD2

V [1]

S* R10* P* B2-* B1* B3* TM3* E3* C5* TM2* I11* H2* C9* E1* I210* I27* I36*I19* I42* TD3* S6* H7* R8* I410* I34* S7* I49* I310* C7* I12* TD2* TD4

V [1]

S* R10* P* B2-* B1* B3* I13* TM3* E3* C5* I28* E4* S5* TM2* I110* TD1* I11*H2* C9* E1* I210* I27* I36* S2* TD9* I43* H3* C3* R8* R2* H4* I410* I34* S7*I310* TD4

V [1]

S* R10* P* B2-* I13* TM3* E3* C5* I28* E4* S5* TM2* I110* TD1* I27* I36* S2*TD9* I43* H3* C3* R2* H4* I410* I34*~{B1* B3* I46* TD6* TM5* H5* I17* I38}*~{B1* B3* I11* S8* H2* C9* E1* I48* I39* I210}*~{B1* B3* H5* I17* I38* I48*R8* TD8* E5* TM6* S4}

V [1]

S* R10* P* B2-* B1* B3* I13* TM3* E3* C5* E4* TM2* I11* H2* C9* E1* I210* I27*I36* S2* I19* I42* TD3* S6* H7* TD9* C3* R8* R2* H4* I410* I34* S7* I310* TD4

V [1]

S* R10* P* B2-* B1* B3* I13* TM3* E3* C5* I28* E4* S5* TM2* I11* C6* H2* C9*E1* I48* I210* I27* I36* R3* I19* I42* TD3* S6* H7* H3* R8* TD8* I410* TM1*S7* I310* TD4

V [1]

S* R10* P* B2-* I13* TM3* E3* C5* I28* E4* S5* C6* H2* C9* I48* I27* I36* R3*H3* TD8* TM1*~{B1* B3* TM2* TD1* I11* S8* E1* I39* I210* I19* I42* TD3* S6*H7}

V [1]

S* R10* P* B2-* B1* B3* I13* TM3* E3* C5* E4* TM2* TD1* I11* S8* H2* C9* E1*I48* I39* I210* I27* I36* S2* I19* I42* TD3* S6* H7* TD9* C3* R2* H4* I410*I34

V [1]

S* R10* P* B2-* B1* B3* TM3* E3* C5* TM2* TD1* I11* S8* H2* C9* E1* I48* I39*I210* I27* I36* I19* I42* TD3* S6* H7* R8* I34* S7* I49* C7* I12* TD2

V [1]

S* R10* P* B2-* I13* TM3* I46* E3* C5* I28* S5* TM2* I110* TD1* E2* TD5* S8*I35* C6* H2* E1* I39* I36* I19* I47* I43* H3* R8* B2* S7* I25* C1

Concept FOR CLASS a-$LiFeO_2$:

[3]

S* R10* P* B2-* B1* B3* TM2* I11* E2* H1* H2* C9* I210* S2* C3* TD8* TM1* I49*I111* S12* B6* I310* R4*~{I13* I28* E4* S5* C6* I48* I36* R3* H3}*~{I17* I38*C6* R3* I26* I47* E8* TD9* H8* D* TM7}*~{I13* TM3* E4* I27* TD9* R2* H4* I410*I34}

V [3]

S* R10* P* B2-* B1* B3* H1* C9* I210* TM1* I49* I111* S12* B6* I310*~{TD1*I11}*~{C5* I28* E4* S5}*~{TM2* TD1* I11* S8* H2* E1* I48* I39}*~{TD8}*~{E3*TM2* I11* H2* E1* I27* R8* I410* I34* S7* C7* I12* TD2* TD4}*~{I17* I38* TM2*I11* C6* H2* E1* S2* R3* I26* I47* E8* TD9* H8* D* TM7* R8* I410* S7* TD4}*~{I13* TM3* E4* TM2* I11* H2* E1* I27* S2* TD9* C3* R8* R2* H4* I410* I34*S7* TD4}*~{I17* TM2* I11* H2* E1* S2* R3* I26* I47* E8* TD9* D* TM7* C3* R8*I410* S7* TD4* H6* I37}*~{TM2* I11* I35* H2* E1* S2* I47* D* TM7* R8* I410*S7* I25* R4* TD4* C4* I18* E7* TD10* H6}

V [1]

S* R10* P* B2-* B1* B3* E3* TM2* I11* E2* H1* H2* C9* I210* I27* S2* C3* R8TD8* I34* TM1* S7* I49* I111* S12* B6* I310* C7* I12* TD2* R4

V [1]

S* R10* P* B2-* B1* B3* I13* TM3* I46* I28* TM2* TD1* I11* E2* R9* H1* S8*I35* C6* H2* C9* I210* S2* C3* TD8* TM1* I49* I111* S12* B6* I310* R4

V [1]

S* R10* P* B2-* I13* TM3* I28* C6* H2* C9* TD8* TM1*~{E3* C5* E4* S5* I110*TD1* I48* I27* I36* I19* I42* TD3* S6* H7* H3* B2* S10* I4~ I37}*~{B1* B3*E3* C5* E4* S5* TM2* TD1* I11* S8* E1* I48* I39* I210* I27* I36* R3* I19* I42*TD3* S6* H7* H3}*~{B1* B3* E3* C5* E4* S5* TM2* I11* E1* I48* I210* I27* I36*R3* I19* I42* TD3* S6* H7* H3* R8* I410* S7* I310* TD4}

V [1]

S* R10* P* B2-* B1* B3* I13* TM3* I46* I28* TD1* E2* R9* H1* S8* I35* C6* H2*C9* TM1*~{TD6* TM5* H5* C5* E4* S5* I17* I38* I210* I49* I111* S12* B6* I310}*~{I38* I11* I29* E1* I210* I49* I111* S12* B6* I310* S10* C10* I44}*~{TM2*I11* E1* I210* R8* I410* S7* I49* I111* S12* B6* I310* TD4}*~{TM2* I11* E1*I48* I39* I210* I49* I111* S12* B6* I310}*~{TM2* I11* I29* E1* I39* I210* I47*I49* I111* S12* B6* I310* S10}

V [1]

S* R10* P* B2-* B1* B3* I13* TM3* I46* I28* TD1* I11* E2* R9* H1* S8* I35* C6*H2* C9* I210* TM1* I111* S12* B6* I310*~{E1}*~{TM2* E1* R8* I410* S7* I49*TD4}

Concept FOR CLASS another structure :

[10]

S* R10* P* B2-* B1* B3* E3* I28* S5* TD1* I36* H3*~{C5* TM2* I110* I35* S2*I47* D* TM7* I43* I25* R4* C4* I18* E7* TD10* H6}*~{I13* TM3* I46* TD6* TM5*H5* C5* E4* I17* I38* TM2* I110* E2* R9* S8* I35* C6* H2* I43}*~{I46* TD6*TM5* H5* C5* E4* I17* I38* TM2* I110* H2* I27* I43* R8* I34* S7* I49* C7* I12*TD2}*~{I46* TD6* TM5* H5* C5* E4* I17* I38* TM2* I110* C6* S2* R3* I26* I47*E8* TD9* H8* D* TM7* I43}*~{I13* TM3* I46* H5* C5* I17* I38* TM2* I110* E2*R9* S8* I35* C6* H2* I48* I43* C3* R8* TD8* E5* TM6* S4}*~{I13* TM3* I46* TD6*TM5* H5* C5* E4* I17* I38* TM2* I110* I27* S2* TD9* I43* C3* R2* H4* I410*I34}*~{I13* I46* TD6* TM5* H5* C5* E4* I17* I38* TM2* I110* C6* I48* R3* I43*TD8* TM1}*~{H5* C5* I17* I38* TM2* I110* H2* I48* I27* I43* C3* R8* TD8* E5*TM6* S4* I34* S7* I49* C7* I12* TD2}*~{I13* H5* C5*

E4* I17* I38* TM2* I110*C6* I48* R3* I43* C3* R8* TD8* E5* TM6* S4* TM1}*~{I13* TM3* H5* C5* E4* I17*I38* TM2* I110* I48* I27* S2* TD9* I43* C3* R8* TD8* E5* TM6* S4* R2* H4*I410* I34}*~{C5* TM2* I110* I11* E2* H2* I210* I27* S2* I43* C3* R8* TD8* I34*S7* I49* I310* C7* I12* TD2* R4}*~{I13* TM3* C5* E4* TM2* I110* I11* H2* C9*E1* I210* I27* S2* TD9* I43* C3* R8* R2* H4* I410* I34* S7* I310* TD4}*~{C5*TM2* I110* I11* H2* C9* E1* I210* I27* I43* R8* I410* I34* S7* I49* I310* C7*I12* TD2* TD4}

V [10]

S* R10* P* B2-* B1* B3* E3* I28* S5* TD1* H3*~{I48* I36}*~{C5* TM2* I110* I35*I36* S2* I47* D* TM7* I43* I25* R4* C4* I18* E7* TD10* H6}*~{I13* TM3* I46*TD6* TM5* H5* C5* E4* I17* I38* TM2* I110* E2* R9* S8* I35* C6* H2* I36* I43}*~{I46* TD6* TM5* H5* C5* E4* I17* I38* TM2* I110* H2* I27* I36* I43* R8* I34*S7* I49* C7* I12* TD2}*~{I46* TD6* TM5* H5* C5* E4* I17* I38* TM2* I110* C6*I36* S2* R3* I26* I47* E8* TD9* H8* D* TM7* I43}*~{I13* TM3* I46* H5* C5* I17*I38* TM2* I110* E2* R9* S8* I35* C6* H2* I48* I36* I43* C3* R8* TD8* E5* TM6*S4}*~{I13* TM3* I46* TD6* TM5* H5* C5* E4* I17* I38* TM2* I110* I27* I36* S2*TD9* I43* C3* R2* H4* I410* I34}*~{I13* I46* TD6* TM5* H5* C5* E4* I17* I38*TM2* I110* C6* I48* I36* R3* I43* TD8* TM1}*~{H5* C5* I17* I38* TM2* I110* H2*I48* I27* I36* I43* C3* R8* TD8* E5* TM6* S4* I34* S7* I49* C7* I12* TD2}*~{I13* H5* C5* E4* I17* I38* TM2* I110* C6* I48* I36* R3* I43* C3* R8* TD8* E5*TM6* S4* TM1}*~{I13* TM3* H5* C5* E4* I17* I38* TM2* I110* I48* I27* I36* S2*TD9* I43* C3* R8* TD8* E5* TM6* S4* R2* H4* I410* I34}*~{C5* TM2* I110* I11*E2* H2* I210* I27* I36* S2* I43* C3* R8* TD8* I34* S7* I49* I310* C7* I12*TD2* R4}*~{I13* TM3* C5* E4* TM2* I110* I11* H2* C9* E1* I210* I27* I36* S2*TD9* I43* C3* R8* R2* H4* I410* I34* S7* I310* TD4}*~{C5* TM2* I110* I11* H2*C9* E1* I210* I27* I36* I43* R8* I410* I34* S7* I49* I310* C7* I12* TD2* TD4}

V [8]

S* R10* P* B2-* I13* TM3* I28*~{TD1}*~{I27* S2* TD9* C3* R2* H4* I410* I34}*~{H2* C9* TM1}*~{B1* B3* I46* E3* TD6* TM5* H5* C5* E4* S5* I17* I38* C6*I48* I27* I36* R3* I19* I42* TD3* S6* H7* H3* TD8* TM1}*~{B1* B3* E3* H5* C5*E4* S5* I17* I38* C6* I48* I27* I36* R3* I19* I42* TD3* S6* H7* H3* C3* R8*TD8* E5* TM6* S4* TM1}*~{E3* C5* E4* S5* I110* E2* C6* I48* I39* I27* I36*I19* I42* TD3* S6* H7* I26* H3* TD8* TM1* B2* C1* R6* TD7}*~{E3* C5* E4* S5*TD5* C6* E1* I48* I39* I27* I36* I19* I42* TD3* S6* H7* I47* H3* R8* TD8* TM1*B2* S7* I25* C1}

V [8]

S* R10* P* B2-* B1* B3* TM2* H2* I49*~{I410}*~{E3* I27* R8* I34* S7* C7* I12*TD2}*~{E3* E1* I27* R8* I34* S7* C7* I12* TD2}*~{C3}*~{TD1* I11* C9* I39*I210* I310}*~{I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17* I38* H1* C9* I210*I27* R8* I34* TM1* S7* I111* S12* B6* I310* C7* I12* TD2}*~{E3* TD1* I11* H1*S8* C9* E1* I48* I39* I210* I27* R8* I34* TM1* S7* I111* S12* B6* I310* C7*I12* TD2}*~{E3* TD1* I11* I29* H1* C9* E1* I39* I210* I27* I47* R8* I34* TM1*S7* I111* S12* B6* I310* C7* I12* TD2* S10}*~{TM3* E3* C5* TD1* I11* S8* C9*E1* I48* I39* I210* I27* I36* I19* I42* TD3* S6* H7* R8* I34* S7* C7* I12*TD2}

V [8]

S* R10* P* B2-* B1* B3* H2* I49*~{TM2* I410}*~{E3* TM2* I27* R8* I34* S7* C7*I12* TD2}*~{I38}*~{E3* TM2* E1* I27* R8* I34* S7* C7* I12* TD2}*~{TM2* C3}*~{TM2* TD1* I11* C9* I39* I210* I310}*~{I46* E3* TD6* TM5* H5* C5* I28* E4*S5* I17* I38* TM2* H1* C9* I210* I27* R8* I34* TM1* S7* I111* S12* B6* I310*C7* I12* TD2}*~{E3* TM2* TD1* I11* H1* S8* C9* E1* I48* I39* I210* I27* R8*I34* TM1* S7* I111* S12* B6* I310* C7* I12* TD2}*~{E3* TM2* TD1* I11* I29* H1*C9* E1* I39* I210* I27* I47* R8* I34* TM1* S7* I111* S12* B6* I310*

C7* I12*TD2* S10}*~{TM3* E3* C5* TM2* TD1* I11* S8* C9* E1* I48* I39* I210* I27* I36*I19* I42* TD3* S6* H7* R8* I34* S7* C7* I12* TD2}
V [7]
S* R10* P* B2-* TM3* I110*~{S5* E2* H1* C9* I48* I39* I210* S2* I26* D* TM7*H3* TM1* B2* C1* I49* I111* S12* B6* I310* R6* TD7}*~{B1* B3* I13* I46* E3*H5* I28* I17* I38* TM2* TD1* E2* C2* I45* TD5* S3* R9* I29* H1* S8* I35* C6*H2* I48* C3* R8* TD8* E5* TM6* S4}*~{B1* B3* I13* I46* E3* TD6* TM5* H5* C5*I28* E4* S5* I17* I38* TM2* TD1* E2* R9* S8* I35* C6* H2* I36* I43* H3}*~{B1*B3* I13* I46* E3* H5* C5* I28* S5* I17* I38* TM2* TD1* E2* R9* S8* I35* C6*H2* I48* I36* I43* H3* C3* R8* TD8* E5* TM6* S4}*~{B1* B3* I13* I46* E3* TD6*TM5* H5* C5* I28* E4* S5* I17* I38* TM2* TD1* I27* I36* S2* TD9* I43* H3* C3*R2* H4* I410* I34}*~{B1* B3* I13* E3* H5* C5* I28* E4* S5* I17* I38* TM2* TD1*I48* I27* I36* S2* TD9* I43* H3* C3* R8* TD8* E5* TM6* S4* R2* H4* I410* I34}*~{I13* E3* C5* I28* E4* S5* TM2* TD1* E2* I48* I39* I27* I36* S2* I26* TD9*I43* H3* C3* H4* I410* I34* B2* C1* R6* TD7}*~{I13* E3* C5* I28* E4* S5* E2*C6* I48* I39* I27* I36* I19* I42* TD3* S6* H7* I26* H3* TD8* TM1* B2* C1* R6*TD7}*~{I13* E3* C5* I28* E4* S5* TD1* C6* H2* C9* I48* I27* I36* I19* I42*TD3* S6* H7* H3* TD8* TM1* B2* S10* I44* I37}*~{I13* I46* E3* C5* I28* S5*TM2* TD1* E2* TD5* S8* I35* C6* H2* E1* I39* I36* I19* I47* I43* H3* R8* B2*S7* I25* C1}*~{B1* B3* I13* E3* H5* I28* E4* I17* I38* TM2* C2* I45* TD5* S3*I29* H1* I48* I27* S2* TD9* C3* R8* TD8* E5* TM6* S4* R2* H4* I410* I34}*~{B1* B3* I13* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17* I38* TM2* C2* I45*TD5* S3* I29* H1* I27* S2* TD9* C3* R2* H4* I410* I34}*~{B1* B3* I13* E3* E4*I38* TM2* I11* E2* C2* I45* TD5* S3* I29* H1* H2* I210* I27* [illegible] TD9* C3* TD8*R2* H4* I410* I34* I310* R4}*~{B1* B3* I13* E3* C5* I28* E4* S5* TM2* TD1*I11* H2* C9* E1* I210* I27* I36* S2* TD9* I43* H3* C3* R8* R2* H4* I410* I34*S7* I310* TD4}*~{I13* E3* E4* S5* I38* TM2* E2* C2* I45* TD5* S3* I29* H1*I48* I39* I27* S2* I26* TD9* H3* C3* H4* I410* I34* B2* C1* R6* TD7}*~{I13*E3* C5* E4* S5* E2* I48* I39* I27* I36* S2* I19* I42* TD3* S6* H7* I26* TD9*H3* C3* H4* I410* I34* B2* C1* R6* TD7}*~{I13* I46* E3* C5* I28* S5* TD1* E2*S8* I35* C6* H2* I48* I39* I27* I36* I19* I42* TD3* S6* H7* I26* H3* B2* C1*R6* TD7}*~{I13* I46* E3* I28* S5* I38* TM2* TD1* E2* C2* I45* TD5* S3* I29*H1* S8* I35* C6* H2* I48* I39* I26* H3* B2* C1* R6* TD7}*~{I13* I46* E3* C5*I28* S5* TM2* TD1* E2* S8* I35* C6* H2* C9* I27* I36* I43* H3* TM1* B2* S10*I44* I37}
V [7]
S* R10* P* B2-* B1* B3* TD1* I11* H1* C9* I210* TM1* I49* I111* S12* B6* I310*~{E3* TM2* S8* H2* E1* I48* I39* I27* R8* I34* S7* C7* I12* TD2}*~{E3* TM2*I29* H2* E1* I39* I27* I47* R8* I34* S7* C7* I12* TD2* S10}*~{I13* TM3* I46*I28* I38* E2* R9* I29* S8* I35* C6* H2* E1* S10* C10* I44}*~{I13* TM3* I46*I28* TM2* E2* R9* S8* I35* C6* H2* E1* R8* I410* S7* TD4}*~{I13* TM3* I46*I28* TM2* E2* R9* S8* I35* C6* H2* E1* I48* I39}*~{I13* TM3* I46* I28* TM2*E2* R9* I29* S8* I35* C6* H2* E1* I39* I47* S10}*~{I13* TM3* I46* I28* TM2*E2* R9* S8* I35* C6* H2* S2* C3* TD8* R4}
V [7]
S* R10* P* B2-* I13* I28* I36*~{E3* C5* E4* S5* I27}*~{E4* S5* C6* I48* R3*H3* TD8* TM1}*~{B1* B3* TM3* I46* E3* H5* C5* I17* I38* TD1* E2* R9* S8* I35*C6* H2* I48* I27* I19* I42* TD3* S6* H7* C3* R8* TD8* E5* TM6* S4}*~{B1* B3*TM3* I46* E3* TD6* TM5* H5* C5* E4* S5* I17* I38* TM2* I110* TD1* E2* R9* S8*I35* C6* H2* I43* H3}*~{B1* B3* TM3* I46* E3* H5* C5* S5* I17* I38* TM2* I110*TD1* E2* R9* S8* I35* C6* H2* I48* I43* H3* C3* R8* TD8* E5* TM6* S4}*~{B1*B3* TM3* E3* H5* C5* E4* I17* I38* I48* I27* S2* I19* I42* TD3* S6* H7* TD9*C3* R8* TD8* E5* TM6* S4* R2* H4* I410* I34}*~{TM3* I46* E3* C5* S5* TM2*I110* TD1* E2* TD5* S8* I35* C6* H2* E1*

I39* I19* I47* I43* H3* R8* B2* S7*I25* C1}*~{TM3* I46* E3* C5* S5* I110* TD1* E2* S8* I35* C6* H2* I48* I39*I27* I19* I42* TD3* S6* H7* I26* H3* B2* C1* R6* TD7}*~{TM3* I46* E3* C5* S5*TM2* I110* TD1* E2* S8* I35* C6* H2* C9* I27* I43* H3* TM1* B2* S10* I44* I37}

V [6]

S* R10* P* B2-* I13* TM3* I27*~{E3* C5* I28* E4* S5* I48* I36* H3}*~{S2* TD9*C3* R2* H4* I410* I34}*~{B1* B3* I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17*I38* TD1* E2* R9* S8* I35* C6* H2* I36* I19* I42* TD3* S6* H7}*~{B1* B3* I46*E3* H5* C5* I28* I17* I38* TD1* E2* R9* S8* I35* C6* H2* I48* I36* I19* I42*TD3* S6* H7* C3* R8* TD8* E5* TM6* S4}*~{E3* E4* S5* I38* TM2* I110* E2* C2*I45* TD5* S3* I29* H1* I48* I39* S2* I26* TD9* H3* C3* H4* I410* I34* B2* C1*R6* TD7}*~{E3* C5* E4* S5* I110* E2* I48* I39* I36* S2* I19* I42* TD3* S6* H7*I26* TD9* H3* C3* H4* I410* I34* B2* C1* R6* TD7}*~{I46* E3* C5* I28* S5*I110* TD1* E2* S8* I35* C6* H2* I48* I39* I36* I19* I42* TD3* S6* H7* I26* H3*B2* C1* R6* TD7}*~{I46* E3* I28* TD1* H2* C9* TM1* S10* I44* I37}

V [6]

S* R10* P* B2-* B1* B3* E3* TM2* I110* I35* S2* I47* D* TM7* I25* R4* C4* I18*E7* TD10* H6*~{C5* I28* S5* TD1* I36* I43* H3}*~{H5* I28* I17* I38* C2* I45*TD5* S3* I29* H1* I48* C3* R8* TD8* E5* TM6* S4}*~{I46* TD6* TM5* H5* C5* I28*E4* S5* I17* I38* C2* I45* TD5* S3* I29* H1}

V [5]

S* R10* P* B2-* I13* TM3* I46* I28* TD1* E2* S8* I35* C6* H2*~{E3* TM2* I110*B2}*~{B1* B3* E3* H5* I17* I38* TM2* I110* C2* I45* TD5* S3* R9* I29* H1* I48*C3* R8* TD8* E5* TM6* S4}*~{B1* B3* E3* TD6* TM5* H5* C5* E4* S5* I17* I38*R9* I27* I36* I19* I42* TD3* S6* H7}*~{B1* B3* E3* H5* C5* I17* I38* R9* I48*I27* I36* I19* I42* TD3* S6* H7* C3* R8* TD8* E5* TM6* S4}*~{B1* B3* E3* TD6*TM5* H5* C5* E4* S5* I17* I38* TM2* I110* R9* I36* I43* H3}*~{B1* B3* E3* H5*C5* S5* I17* I38* TM2* I110* R9* I48* I36* I43* H3* C3* R8* TD8* E5* TM6* S4}*~{E3* C5* S5* TM2* I110* TD5* E1* I39* I36* I19* I47* I43* H3* R8* B2* S7*I25* C1}*~{B1* B3* R9* H1* C9* TM1}*~{B1* B3* I11* R9* H1* C9* I210* TM1*I111* S12* B6* I310}*~{E3* C5* S5* I110* I48* I39* I27* I36* I19* I42* TD3*S6* H7* I26* H3* B2* C1* R6* TD7}

V [4]

S* R10* P* B2-* B1* B3* E3* TM2* I110* H2* E1* I27* R8* I34* S7* I49* C7* I12*TD2*~{I38* I11* C2* I45* TD5* S3* I29* H1* C9* I210* I410* I310* TD4}*~{C5*I28* S5* TD1* I11* C9* I210* I36* I43* H3* I410* I310* TD4}

V [4]

S* R10* P* B2-* B1* B3* TM2* TD1* I11* H1* S8* H2* C9* E1* I48* I39* I210*TM1* I49* I111* S12* B6* I310*~{E3* I27* R8* I34* S7* C7* I12* TD2}*~{I13*TM3* I46* I28* E2* R9* I35* C6}

V [3]

S* R10* P* B2-* B1* B3* I13* TM3* I46* E3* I28* I38* TM2* I110* TD1* I11* E2*C2* I45* TD5* S3* R9* I29* H1* S8* I35* C6* H2

V [3]

S* R10* P* B2-* B1* B3* I38* TM2* I110* C2* I45* TD5* S3* I29* H1* H2* I49*~{E3* H5* I28* I17* I48* I27* C3* R8* TD8* E5* TM6* S4* I34* S7* C7* I12*TD2}*~{I46* E3* TD6* TM5* H5* C5* I28* E4* S5* I17* I27* R8* I34* S7* C7* I12*TD2}*~{E3* I11* C9* E1* I210* I27* R8* I410* I34* S7* I310* C7* I12* TD2* TD4}

V [2]

S* R10* P* B2-* B1* B3* H1* C9* I210* TD8* TM1* I49* I111* S12* B6* I310*~{C3* R8}*~{I11* H2}*~{I13* TM3* H5* I28* E4* I17* I38* I48* I27* S2* TD9* C3*R8* E5* TM6* S4* R2* H4* I410* I34}*~{I13* I28* E4* S5* TM2* I11*

C6* H2* E1*I48* I36* R3* H3* R8* I410* S7* TD4}*~{I13* I46* TD6* TM5* H5* C5* I28* E4*S5* I17* I38* C6* I48* I36* R3* H3}
V [2]
S* R10* P* B2-* B1* B3* E3* C3*~{R8* TD8}*~{S2* I34}
V [2]
S* R10* P* B2-* I13* E4* S5* H1* C6* H2* C9* I48* R3* H3* TD8* TM1*~{B1* B3*I28* TM2* I11* E2* I210* I36* S2* C3* I49* I111* S12* B6* I310* R4}*~{B1* B3*I28* TM2* I11* E1* I210* I36* R8* I410* S7* I49* I111* S12* B6* I310* TD4}
V [2]
S* R10* P* B2-* B1* B3* TM2* TD1* I11* H1* S8* H2* C9* E1* I48* I39* I210*I47* TM1* I49* I111* S12* B6* I310
V [2]
S* R10* P* B2-* B1* B3* TM2* TD1* I11* H1* S8* H2* C9* E1* I48* I39* I210* C3*TM1* I49* I111* S12* B6* I310
V [2]
S* R10* P* B2-* I13* TM3* I46* E3* I28* I38* TM2* I110* TD1* E2* C2* I45* TD5*S3* I29* H1* S8* I35* C6* H2* B2*~{S5* I48* I39* I26* H3* C1* R6* TD7}
V [1]
S* R10* P* B2-* B1* B3* E3* C5* I28* S5* I17* I38* TM2* I110* TD1* I11* C6*H2* C9* E1* I210* I36* S2* R3* I26* I47* E8* TD9* H8* D* TM7* I43* H3* R8*I410* S7* I310* TD4
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* E4* TM2* TD1* I11* H1* S8* H2* C9* E1* I48*I39* I210* I27* S2* TD9* C3* R2* H4* I410* I34* TM1* I49* I111* S12* B6* I310
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* E3* C5* I28* E4* S5* TM2* TD1* I11* S8* C6*H2* C9* E1* I48* I39* I210* I27* I36* R3* I19* I42* TD3* S6* H7* H3* TD8* TM1
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* E4* I38* TD1* I11* I29* H1* C9* E1* I210*I27* S2* TD9* C3* R2* H4* I410* I34* TM1* I49* I111* S12* B6* I310* S10* C10*I44
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* I46* TD6* TM5* H5* C5* I28* E4* S5* I17*I38* H1* C9* I210* I27* S2* TD9* C3* R2* H4* I410* I34* TM1* I49* I111* S12*B6* I310
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* E3* C5* I28* E4* S5* TM2* I110* TD1* I11*S8* H2* C9* E1* I48* I39* I210* I27* I36* S2* TD9* I43* H3* C3* R2* H4* I410*I34
V [1]
S* R10* P* B2-* B1* B3* I13* E3* I28* E4* S5* I38* TM2* I110* TD1* I11* C2*I45* TD5* S3* I29* H1* S8* C6* H2* C9* E1* I48* I39* I210* I36* R3* H3* TD8*TM1
V [1]
S* R10* P* B2-* B1* B3* I13* E3* C5* I28* E4* S5* TM2* I110* TD1* I11* S8* C6*H2* C9* E1* I48* I39* I210* I36* R3* I43* H3* TD8* TM1
V [1]
S* R10* P* B2-* B1* B3* I13* I28* E4* S5* TM2* TD1* I11* H1* S8* C6* H2* C9*E1* I48* I39* I210* I36* R3* H3* TD8* TM1* I49* I111* S12* B6* I310
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* I46* E3* I28* I38* TM2* I110* TD1* I11*

E2*C2* I45* TD5* S3* R9* I29* H1* S8* I35* C6* H2* C9* E1* I48* I39* I210
V [1]
S* R10* P* B2-* B1* B3* E3* C5* I28* S5* TM2* I110* TD1* I11* S8* I35* H2* C9*E1* I48* I39* I210* I36* S2* I47* D* TM7* I43* H3* I25* R4* C4* I18* E7* TD10*H6
V [1]
S* R10* P* B2-* B1* B3* I17* TM2* TD1* I11* H1* S8* H2* C9* E1* I48* I39*I210* S2* R3* I26* I47* E8* TD9* D* TM7* C3* TM1* I49* I111* S12* B6* I310*H6* I37
V [1]
S* R10* P* B2-* B1* B3* I13* I28* E4* S5* TM2* TD1* I11* I29* H1* C6* C9* E1*I48* I39* I210* I36* R3* I47* H3* TD8* TM1* I49* I111* S12* B6* I310* S10
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* I46* E3* I28* I38* TM2* I110* TD1* I11* E2*C2* I45* TD5* S3* R9* I29* H1* S8* I35* C6* H2* C9* E1* I39* I47* S10
V [1]
S* R10* P* B2-* B1* B3* E3* C5* I28* S5* TM2* I110* TD1* I11* I29* H1* I35*C9* E1* I39* I36* S2* I47* D* TM7* I43* H3* I25* R4* S10* C4* I18* E7* TD10*H6
V [1]
S* R10* P* B2-* B1* B3* I13* E3* I28* E4* S5* I38* TM2* I110* TD1* I11* C2*I45* TD5* S3* I29* H1* C6* E1* I48* I36* R3* H3* TD8* TM1* S10* C10* I44
V [1]
S* R10* P* B2-* B1* B3* I13* TM3* I46* E3* I28* I38* TM2* I110* TD1* I11* E2*C2* I45* TD5* S3* R9* I29* H1* S8* I35* C6* H2* E1* TM1* S10* C10* I44
V [1]
S* R10* P* B2-* B1* B3* E3* C5* I28* S5* I38* TM2* I110* TD1* I11* I29* H1*I35* E1* I36* S2* I47* D* TM7* I43* H3* TM1* I25* R4* S10* C10* I44* C4* I18*E7* TD10* H6
V [1]
S* R10* P* B2-* B1* B3* E3* H5* I28* I17* I38* TM2* I110* C2* I45* TD5* S3*I29* H1* C6* I48* S2* R3* I26* I47* E8* TD9* H8* D* TM7* C3* R8* TD8* E5* TM6*S4
V [1]
S* R10* P* B2-* I13* TM3* I46* E3* I28* I38* TM2* I110* TD1* E2* C2* I45* TD5*S3* I29* H1* S8* I35* C6* H2* C9* I27* TM1* B2* S10* I44* I37
V [1]
S* R10* P* B2-* B1* B3* E3* C5* I28* S5* TM2* I110* TD1* I11* S8* H2* C9* E1*I48* I39* I210* I27* I36* I43* H3* R8* I34* S7* I49* C7* I12* TD2
V [1]
S* R10* P* B2-* I13* TM3* I46* E3* I28* I38* TM2* I110* TD1* E2* C2* I45* TD5*S3* I29* H1* S8* I35* C6* H2* E1* I39* I19* I47* H3* R8* B2* S7* I25* C1

Concept FOR CLASS without compound ABX_2 :

[3]
S* R10* P* B2-* TM3* S5* I110* E2* H1* C9* I48* I39* I210* S2* I26* D* TM7*H3* TM1* B2* C1* I49* I111* S12* B6* I310* R6* TD7
V [2]
S* R10* P* B2-* I13* TM3* I46* E3* I28* TM2* I110* TD1* E2* S8* I35* C6* H2*B2*~{I38* C2* I45* TD5* S3* I29* H1}*~{C5* S5* TD5* E1* I39* I36* I19* I47*I43* H3* R8* S7* I25* C1}
V [1]
S* R10* P* B2-* I13* TM3* I46* E3* I28* S5* I38* TM2* I110* TD1* E2* C2*

I45*TD5* S3* I29* H1* S8* I35* C6* H2* I48* I39* I26* H3* B2* C1* R6* TD7
V [1]
S* R10* P* B2-* I13* TM3* I46* E3* C5* I28* S5* TM2* I110* TD1* E2* S8*
I35*C6* H2* C9* I27* I36* I43* H3* TM1* B2* S10* I44* I37
V [1]
S* R10* P* B2-* I13* TM3* I46* E3* I28* TD1* H2* C9* I27* TM1* S10* I44*
I37*~{I38* TM2* I110* E2* C2* I45* TD5* S3* I29* H1* S8* I35* C6* B2}

Appendix 3

Appendix 3

Logical Expressions for Predicting Crystal Types for Composition ABX_2

Feature set I (with alterations)

Concept FOR CLASS chalcopyrite :

[17]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*~{P36*D310* S42}*~{R2}*~{P40}

V [17]
P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*~{D40* S50* P36*D310* S42}*~{D40* S50* R2}*~{P36* D310* S42* R5* P52* R4* P46* D410* S52}*~{D40* S50* P40}*~{P36* D310* S42* P52* R4* P46* D410* S52* P56* S62* F414*D510* R6}*~{D40* S50* P36* D310* S42* P40* P52* R4* P46* D410* S52* P56* S62*R10* P34* D30* S40* R1}*~{D40* S50* P36* D310* S42* P40* P52* R4* P46* D410*S52* D30* S40* P53* P30}*~{D40* S50* P36* D310* S42* P40* P52* R4* P46* D410*S52* P56* S62* F414* D510* D30* S40* P30* P63* R8}*~{D40* S50* P36* D310* S42*P40* P52* R4* P46* D410* S52* P34* D30* S40* R1* B2}*~{D40* S50* P36* D310*S42* R2* P40* P52* R4* P46* D410* S52* P44* R3}*~{D40* S50* P36* D310* S42*P40* P52* R4* P46* D410* S52* R3* P54}

V [10]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* R2* P40*~{D30* S40}*~{P36* D310* S42* P42}*~{P36* D310* S42* P52* R4* P46* D410* S52*P44* R3}

V [7]
R5* P46* D410* S52*~{P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60*S70* P36* D310* S42* P52* R4}*~{D40* S50* P50* S12* S22* P26* S32* F40* D50*F50* S60* P60* D60* S70* R2}*~{D40* S50* P50* S12* S22* P26* S32* F40* D50*F50* S60* P60* D60* S70* P36* D310* S42* P40* P52* R4* P34* D30* S40* R1}*~{D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* P36*D310* S42* R2* P44* P42}

V [6]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* P36*D310* S42* P42*~{R2* P40}*~{P44}*~{R2* P40* D30* S40* R1* P30* S30* P23}*~{R2* P40* R4* D30* S40* R1* P30* P33}*~{R2* R4* P46* D410* S52* P56* S62* F414*D510* R6* P54}

V [6]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* P36*D310* S42* R4* P46* D410* S52*~{P52}*~{P54}*~{R2* P40* D30* S40* P32}*~{P40*P52* R3* P54}*~{R2* P40* R3* P54* P42}

V [6]
P36* D310* S42* P43

V [5]
P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* P36* D310* S42*P52* R4*~{R5* P46* D410* S52}*~{P46* D410* S52* P56* S62* F414* D510* R6}*~{D40* S50* P40* P46* D410* S52* P56* S62* R10* P34* D30* S40* R1}*~{D40* S50*P40* P46* D410* S52* D30* S40* P53* P30}*~{D40* S50* P40* P46* D410* S52* P56*S62* F414* D510* D30* S40* P30* P63* R8}*~{D40* S50* P40* P46* D410* S52* P34*D30* S40* R1* B2}*~{D40* S50* R2* P40* P46* D410* S52* P44* R3}*~{D40* S50*P40* P46* D410* S52* R3* P54}

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  V [4]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* P40* P52* R4* P46* D410* S52*~{D30* S40}*~{R3}*~{P56* S62*
R10*P34* D30* S40* R1}
  V [4]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* P40* P52* R4* P46* D410* S52*~{D30* S40}*~{R3}*~{P56* S62*
R10*P34* D30* S40* R1}*~{R5* P34* D30* S40* R1}
  V [2]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* P40*
R1*P30* S30* P23*~{R2* D30* S40}*~{R5* D30* S40* P33* S31}
  V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* R2*
P40*R4* D30* S40* R1* P30* P33* P32
  V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* P40* D30* S40* R1* R3* P33* P32
  V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* P40* R5* P46* D410* S52* D30* S40* R1* P33* P32
  V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* P40* D30* S40* R3* P32* P43
  V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* P40* R5* P46* D410* S52* D30* S40* P32* P43
  V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* P40* D30* S40* R1* R3* P42* P33
  V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* P40* R3* P42* P43
  V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* P40* R5* P46* D410* S52* D30* S40* R1* P42* P33
  V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* P40* D30* S40* R1* P30* B2* P42* S30* P23
  V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* R5* P46* D410* S52* P42* P43
  V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* R5* R4* P46* D410* S52* P54* P42
  V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* P40* P52* R4* P46* D410* S52* D30* S40* R1* R3* P33
  V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* P40* P52* R4* P46* D410* S52* R3* P43
  V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* P40* P52* R4* P46* D410* S52* P53* R3
  V [1]
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D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* P40* R5* P52* R4* P46* D410* S52* D30* S40* R1* P33
V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* R5* P52* R4* P46* D410* S52* P43
V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* R5* P52* R4* P46* D410* S52*~{P44}

Concept FOR CLASS b_$NaFeO_2$:

[3]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* R2*
P40*D30* S40* R1* P30* S30* P23*~{P36* D310* S42* B2* P42}
V [3]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* R2*
P40*D30* S40*~{P36* D310* S42* R4* P46* D410* S52* P32}*~{P36* D310* S42*
R3* P32*P43}*~{P36* D310* S42* R5* P46* D410* S52* P32* P43}*~{P36* D310*
S42* R5*P46* D410* S52* R1* P33* P32}*~{R1* P33}*~{R4* R1* P30* P33*
P32}*~{P36* D310*S42* R1* R3* P33* P32}*~{P36* D310* S42* R1* P30* B2*
P42* S30* P23}*~{P36*D310* S42* P46* D410* S52* P56* S62* F414* D510* R6*
P34* R1* P42}
V [2]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* P40* D30* S40* R1* P30* P42* S30* P23*~{B2}
V [2]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* P40* P42*~{R3* P43}*~{R5* P46* D410* S52* D30* S40*
R1* P33}*~{R4* D30* S40* R1* P30* P33}*~{R4* P46* D410* S52* R3*
P54}*~{D30* S40* R1*R3* P33}*~{D30* S40* R1* P30* B2* S30* P23}*~{P46*
D410* S52* P56* S62* F414*D510* R6* P34* D30* S40* R1}
V [2]
P36* D310* S42* P42*~{D40* S50* P50* S12* S22* P26* S32* F40* D50* F50*
S60*P60* D60* S70}*~{D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60*
P60*D60* S70* R2* P40* R3* P43}*~{D40* S50* P50* S12* S22* P26* S32* F40*
D50*F50* S60* P60* D60* S70* R2* P40* R5* P46* D410* S52* D30* S40* R1*
P33}*~{D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60*
S70* R2* R5*R4* P46* D410* S52* P54}*~{D40* S50* P50* S12* S22* P26* S32*
F40* D50* F50*S60* P60* D60* S70* R2* R5* P46* D410* S52* P43}*~{D40* S50*
P50* S12* S22*P26* S32* F40* D50* F50* S60* P60* D60* S70* R2* R5* P46*
D410* S52* P44}*~{D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60*
P60* D60* S70* R2* P40*R4* P46* D410* S52* R3* P54}*~{D40* S50* P50* S12*
S22* P26* S32* F40* D50*F50* S60* P60* D60* S70* R2* P40* D30* S40* R1*
R3* P33}
V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* P40* R4* D30* S40* R1* P30* P42* S30* P23

Concept FOR CLASS another structure :

[3]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P40*~{P36* D310* S42* R4}*~{R1* P30* S30* P23}*~{P46* D410* S52* P56* S62*
F414*D510* R6* P34* D30* S40* R1}*~{P36* D310* S42* R2* R3* P42*
P43}*~{P36* D310*S42* R2* D30* S40* R3* P32* P43}*~{P36* D310* S42* R2*

R5* P46* D410* S52*D30* S40* P32* P43}*~{P36* D310* S42* R2* R5* P46* D410* S52* D30* S40* R1*P33* P32}*~{P36* D310* S42* R2* R5* P46* D410* S52* D30* S40* R1* P42* P33}*~{R2* R4* D30* S40* R1* P30* P33* P32}*~{P36* D310* S42* R2* D30* S40* R1*R3* P33* P32}*~{P36* D310* S42* R2* D30* S40* R1* R3* P42* P33}

V [1]

D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* P36*D310* S42* R2* P40* R4* D30* S40* R1* P30* P42* P33

V [1]

D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* R2* P40*D30* S40* R1* P33*~{P36* D310* S42* R5* P46* D410* S52* P32}*~{P36* D310* S42*R5* P46* D410* S52* P42}*~{R4* P30* P32}*~{P36* D310* S42* R3* P32}*~{P36*D310* S42* R3* P42}

V [1]

D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* P36*D310* S42* P40* P52* R4* P46* D410* S52* P56* S62* R10* P34* D30* S40* R1

V [1]

D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* P40* R5*D30* S40* R1* P30* S30* P23* P33* S31

Concept FOR CLASS without compounds ABX_2 :

[21]

S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*~{P50}

V [21]

P36* D310* S42*~{D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60*D60* S70* R4* P46* D410* S52}*~{D40* S50* P50* S12* S22* P26* S32* F40* D50*F50* S60* P60* D60* S70* P42}*~{P43}*~{P50* S12* S22* P26* S32* F40* D50* F50*S60* P60* D60* S70* P52* R4}*~{D40* S50* P50* S12* S22* P26* S32* F40* D50*F50* S60* P60* D60* S70* P40* P52* R4* P46* D410* S52}*~{P42}*~{D40* S50* P50*S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* R2* P40* D30* S40* R3*P32* P43}*~{D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60*S70* R2* P40* R5* P46* D410* S52* D30* S40* P32* P43}*~{D40* S50* P50* S12*S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* R2* P40* R5* P46* D410* S52*D30* S40* R1* P33* P32}*~{D40* S50* P50* S12* S22* P26* S32* F40* D50* F50*S60* P60* D60* S70* R2* P40* R4* D30* S40* R1* P30* P42* P33}*~{D40* S50* P50*S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* R2* P40* D30* S40* R1*R3* P33* P32}*~{D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60*D60* S70* R2* P40* R4* D30* S40* R1* P30* P42* S30* P23}

V [21]

P46* D410* S52*~{R5}*~{D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60*P60* D60* S70* P36* D310* S42* R4}

V [16]

D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* P36*D310* S42*~{R4* P46* D410* S52}*~{P42}*~{P40* P52* R4* P46* D410* S52}*~{R2*P40* D30* S40* R3* P32* P43}*~{R2* P40* R5* P46* D410* S52* D30* S40* P32*P43}*~{R2* P40* R5* P46* D410* S52* D30* S40* R1* P33* P32}*~{R2* P40* R4*D30* S40* R1* P30* P42* P33}*~{R2* P40* D30* S40* R1* R3* P33* P32}*~{R2* P40*R4* D30* S40* R1* P30* P42* S30* P23}

V [10]

D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* P36*D310* S42* P40* R4*~{P52* P46* D410* S52}*~{R2* D30* S40* R1* P30*

P42* P33}*~{R2* D30* S40* R1* P30* P42* S30* P23}
V [10]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
R2*~{P40}*~{P36* D310* S42* P40* R5* P46* D410* S52* D30* S40* P32*
P43}*~{P36*D310* S42* P40* R5* P46* D410* S52* D30* S40* R1* P33*
P32}*~{P36* D310* S42*P40* R5* P46* D410* S52* D30* S40* R1* P42*
P33}*~{P36* D310* S42* R5* R4*P46* D410* S52* P54* P42}*~{P36* D310* S42*
R5* P46* D410* S52* P42* P43}*~{P36* D310* S42* R5* P52* R4* P46* D410*
S52}
V [9]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* P52* R4* P46* D410* S52*~{P40}*~{R2* R5}
V [5]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* P40* P52* R4* P46* D410* S52* D30* S40*~{R1* R3*
P33}*~{P56* S62*R10* P34* R1}*~{R5* R1* P33}
V [5]
P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* P36* D310*
S42*R5* P52* R4* P46* D410* S52*~{D40* S50* P40* D30* S40* R1*
P33}*~{D40* S50*R2* P43}
V [4]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R4* P46* D410* S52* P54*~{R2* R5* P42}
V [3]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* R2*
R5*P46* D410* S52*~{P36* D310* S42* P40* D30* S40* P32* P43}*~{P36* D310*
S42*P40* D30* S40* R1* P33* P32}*~{P36* D310* S42* P40* D30* S40* R1*
P42* P33}*~{P36* D310* S42* R4* P54* P42}*~{P36* D310* S42* P42*
P43}*~{P36* D310* S42*P52* R4}
V [2]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P40*P46* D410* S52* P56* S62* F414* D510* R6* P34* D30* S40* R1
V [2]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* P40* R4* P46* D410* S52* D30* S40* P32
V [2]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* P44* P42
V [2]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* P40* P52* R4* P46* D410* S52* R3*~{D30* S40* R1*
P33}*~{R2* P43}*~{P53}
V [2]
P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70* P36* D310*
S42*P52* R4* P46* D410* S52* P56* S62* F414* D510* R6
V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* P40* R4* P46* D410* S52* R3* P54* P42
V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* P40* P46* D410* S52* P56* S62* F414* D510* R6* P34*
D30* S40*R1* P42
V [1]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*

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P36*D310* S42* R2* R4* P46* D410* S52* P56* S62* F414* D510* R6* P54* P42
  V  [ 1 ]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* P40* P52* R4* P46* D410* S52* D30* S40* P53* P30
  V  [ 1 ]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* P40* P52* R4* P46* D410* S52* P56* S62* F414* D510* D30*
S40* P30*P63* R8
  V  [ 1 ]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* P40* P52* R4* P46* D410* S52* P34* D30* S40* R1* B2
  V  [ 1 ]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* P40* P52* R4* P46* D410* S52* P44* R3
  V  [ 1 ]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* P40* P52* R4* P46* D410* S52* R3* P54
  V  [ 1 ]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* R5* P46* D410* S52* P44* P42
  V  [ 1 ]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* P40* R5* P52* R4* P46* D410* S52* P34* D30* S40* R1
  V  [ 1 ]
D40* S50* P50* S12* S22* P26* S32* F40* D50* F50* S60* P60* D60* S70*
P36*D310* S42* R2* R5* P52* R4* P46* D410* S52* P44
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Feature set IV. (with alterations)

Concept FOR CLASS chalcopyrite :

[17]
S* P*~{TM3}*~{E3* C5}*~{C2* TD5* S7* RC8* I36* TM2* I45}*~{H1}*~{S1* C1* H3*E7* TD11* TM7}
V [15]
S* P* TM3* C1* H3*~{TD5* S7* I39}*~{I39* RC7* I110* RC5* I37* E2* E5* TM5*H10* I18* I48* S5* TD8* S3* I25* I44* I26* TD7}*~{E3* C5* C2* RC8* I36* I39*RC7* I110* RC5* I37* E2* E5* TM5* H10* I18* I48* S5* TD8* S3* I25* I44* I26*TD7* I19* I42* TD3* S6* H7* I27}*~{E3* C5* C2* TD5* S7* RC8* I36* TM2* I45*I39* RC7* I110* RC5* E2* I48* S5* I26* TD7* E4* TD1* I28* I43* I16* I24}
V [8]
S* P* TM3* RC7*~{E3* C5* C2* TD5* S7* RC8* I36* TM2* I45* C1* H3* I39* I110*E2* I48* S5* I26* TD7* E4* I16* I24}*~{C1* H3* I39* I110* RC5* I37* E2* E5*TM5* H10* I18* I48* S5* TD8* S3* I25* I44* I26* TD7}
V [5]
S* P* TM3* C2* TD5* S7* RC8* I36* TM2* I45* E4*~{C1* H3* I39* I19* I16* I24*I47* RC9* E1}*~{E3* C5* H3* I110* I37* I44* I27* TD1* I16* I24* H2* S10* C9*TM1}*~{E3* C5* C1* H3* I39* RC7* I110* RC5* E2* I48* S5* I26* TD7* TD1* I28*I43* I16* I24}*~{E3* C5* H3* E2* TD8* S3* I44* I27* I16* I24* I33* H4* TD2*I310* I410* I17* C4* TM4}*~{E3* C5* C1* H3* I39* RC7* I110* E2* I48* S5* I26*TD7* I19* I42* TD3* S6* H7* I27* I16* I24}
V [5]
S* P* TM3* C2* TD5* S7* RC8* I36* TM2* I45* C1* H3* I39* I110* E4* I16* I24*~{E3}*~{E3* H1* S3* I25* I19* I47* RC9* E1* I29* I38* RC4}
V [2]
S* P* C2* H1* I39* C9* TM1* RC2* I111* I210* I49* S12*~{E5* TM5* H10* TD8* S3}*~{TM3* S7* TM2* S1* I110* I27* E4* RC9* E1* H2* I310* I410* RC4* TD4* I11*I46* I35}
V [1]
S* P* TM3* C2* RC8* H1* S1* C1* H3* E7* TD11* TM7* I110* RC5* I37* E2* I18*TD8* S3* I25* I44* I27* E4* I24* H4* I310* I410* I17* C4* TM4* RC4* I46* I35
V [1]
S* P* TM3* C2* H1* S1* C1* H3* E7* TD11* TM7* I39* RC7* I110* RC5* I37* E2*I18* I48* S5* I25* I44* I26* TD7* I27* E4* RC4* I46* I35
V [1]
S* P* TM3* C2* TD5* S7* H1* S1* C1* H3* E7* TD11* TM7* I39* I110* RC5* I37*I18* I25* I44* I19* I27* E4* I47* RC9* E1* RC4* I46* I35
V [1]
S* P* TM3* S1* C1* H3* E7* TD11* TM7* I39* RC7* I110* RC5* I37* E2* H10* I18*I48* S5* I25* I44* I26* TD7* E4* TM4* I46* C3* I34* S4
V [1]
S* P* TM3* TD5* S7* S1* C1* H3* E7* TD11* TM7* I39* I110* RC5* I37* H10* I18*I25* I44* I26* TD7* I19* E4* I47* RC9* E1* TM4* I46* C3* I34* S4
V [1]
S* P* TM3* C2* H1* S1* C1* H3* I39* RC7* I110* RC5* I37* E2* E5* TM5* H10*I18* I48* S5* TD8* S3* I25* I44* I26* TD7* I27* E4* RC4* I46* I35
V [1]
S* P* TM3* C2* TD5* S7* H1* S1* C1* H3* I39* I110* RC5* I37* E5* TM5* H10*I18* TD8* S3* I25* I44* I19* I27* E4* I47* RC9* E1* RC4* I46* I35
V [1]
S* P* TM3* E3* C5* C2* TD5* S7* RC8* I36* C1* H3* I39* RC5* I37* E5* TM5*

H10*I18* TD8* S3* I25* I44* I19* I42* TD3* S6* H7* I27* I47* RC9* E1
V [1]
S* P* TM3* C2* TD5* S7* RC8* I36* TM2* I45* H1* S1* C1* H3* I39* RC7* I110*E2* I48* S5* I26* TD7* I27* E4* I16* I24* RC4* I46* I35
V [1]
S* P* TM3* C2* TD5* S7* RC8* I36* TM2* I45* H1* S1* C1* H3* I39* I110* I25*I19* I27* E4* I16* I24* I47* RC9* E1* RC4* I46* I35
V [1]
S* P* TM3* C2* TM2* H1* S1* I39* RC7* I110* E2* TD8* I27* E4* H2* C9* TM1*I310* RC4* RC2* I111* I210* I49* S12* I11* I46* I35* C3* S2
V [1]
S* P* TM3* C2* C1* H3* I39* RC7* I110* RC5* I37* E2* E5* TM5* H10* I18* I48*S5* TD8* S3* I25* I44* I26* TD7* E4* TM4* I46* C3* I34* S4
V [1]
S* P* TM3* C2* TD5* S7* C1* H3* I39* I110* RC5* I37* E5* TM5* H10* I18* TD8*S3* I25* I44* I26* TD7* I19* E4* I47* RC9* E1* TM4* I46* C3* I34* S4
V [1]
S* P* TM3* C2* TD5* S7* RC8* I36* TM2* I45* C1* H3* I39* I110* RC5* H10* I25*I26* TD7* I19* E4* I16* I24* I47* RC9* E1* TM4* I46* C3* I34* S4
V [1]
S* P* E3* C2* H1* I39* RC5* I37* E5* TM5* H10* I18* S5* TD8* S3* I25* I44* C9*TM1* H4* I310* RC2* I111* I210* I49* S12* TD6* C6* I13* I22

Concept FOR CLASS b_$NaFeO_2$:

[3]
S* P* H1* I39* C9* TM1* RC2* I111* I210* I49* S12*~{C2}
V [3]
S* P* H1*~{TD5* TM2* I45* I29* I38* RC4}*~{I110* E4* RC4* I46}*~{C2* I39* C9*TM1* RC2* I111* I210* I49* S12}*~{TM3* C2* S1* I110* I27* E4* RC4* I46* I35}*~{C2* TD5* TM2* I45* I27* C9* TM1* I29* I38* RC4}*~{TM3* E3* C2* TD5* S7*RC8* I36* TM2* I45* C1* H3* I39* I110* S3* I25* I19* E4* I16* I24* I47* RC9*E1* I29* I38* RC4}
V [2]
S* P* C2* H1* I39* E5* TM5* H10* TD8* S3* C9* TM1* RC2* I111* I210* I49* S12*~{E3* RC5* I37* I18* S5* I25* I44* H4* I310* TD6* C6* I13* I22}
V [1]
S* P* RC8* H1* S1* C1* H3* E7* TD11* TM7* I39* RC5* I37* E2* I18* TD8* S3*I25* I44* I24* C9* TM1* H4* I310* I410* I17* C4* TM4* RC2* I111* I210* I49*S12
V [1]
S* P* TM3* C2* H1* C1* H3* I39* RC7* I110* RC5* I37* E2* E5* TM5* H10* I18*I48* S5* TD8* S3* I25* I44* I26* TD7* C9* TM1* RC2* I111* I210* I49* S12
V [1]
S* P* TM3* C1* H3* I39* RC7* I110* RC5* I37* E2* E5* TM5* H10* I18* I48* S5*TD8* S3* I25* I44* I26* TD7*~{E3* C5* C2* RC8* I36* I19* I42* TD3* S6* H7*I27}*~{C2* H1* S1* I27* E4* RC4* I46* I35}*~{C2* E4* TM4* I46* C3* I34* S4}

Concept FOR CLASS another structure :

[3]
S* P* H1* I110* E4* RC4* I46*~{TM3* C2* RC8* S1* C1* H3* E7* TD11* TM7* RC5*I37* E2* I18* TD8* S3* I25* I44* I27* I24* H4* I310* I410* I17* C4* TM4* I35}*~{TM3* C2* S1* C1* H3* E7* TD11* TM7* I39* RC7* RC5* I37* E2* I18*

I48* S5*I25* I44* I26* TD7* I27* I35}*~{TM3* C2* TD5* S7* S1* C1* H3* E7* TD11* TM7*I39* RC5* I37* I18* I25* I44* I19* I27* I47* RC9* E1* I35}*~{TM3* C2* S1* C1*H3* I39* RC7* RC5* I37* E2* E5* TM5* H10* I18* I48* S5* TD8* S3* I25* I44*I26* TD7* I27* I35}*~{TM3* C2* TD5* S7* S1* C1* H3* I39* RC5* I37* E5* TM5*H10* I18* TD8* S3* I25* I44* I19* I27* I47* RC9* E1* I35}*~{TM3* C2* TM2* S1*I39* RC7* E2* TD8* I27* H2* C9* TM1* I310* RC2* I111* I210* I49* S12* I11*I35* C3* S2}*~{TM3* C2* TD5* S7* RC8* I36* TM2* I45* S1* C1* H3* I39* RC7* E2*I48* S5* I26* TD7* I27* I16* I24* I35}*~{TM3* C2* TD5* S7* RC8* I36* TM2* I45*S1* C1* H3* I39* I25* I19* I27* I16* I24* I47* RC9* E1* I35}

V [2]

S* P* TM3* C2* H1* S1* I110* I27* E4* RC4* I46* I35*~{RC8* C1* H3* E7* TD11*TM7* RC5* I37* E2* I18* TD8* S3* I25* I44* I24* H4* I310* I410* I17* C4* TM4}*~{C1* H3* E7* TD11* TM7* I39* RC7* RC5* I37* E2* I18* I48* S5* I25* I44* I26*TD7}*~{TD5* S7* C1* H3* E7* TD11* TM7* I39* RC5* I37* I18* I25* I44* I19* I47*RC9* E1}*~{C1* H3* I39* RC7* RC5* I37* E2* E5* TM5* H10* I18* I48* S5* TD8*S3* I25* I44* I26* TD7}*~{TD5* S7* C1* H3* I39* RC5* I37* E5* TM5* H10* I18*TD8* S3* I25* I44* I19* I47* RC9* E1}*~{TM2* I39* RC7* E2* TD8* H2* C9* TM1*I310* RC2* I111* I210* I49* S12* I11* C3* S2}*~{TD5* S7* RC8* I36* TM2* I45*C1* H3* I39* RC7* E2* I48* S5* I26* TD7* I16* I24}*~{TD5* S7* RC8* I36* TM2*I45* C1* H3* I39* I25* I19* I16* I24* I47* RC9* E1}

V [1]

S* P* TM3* C2* S7* TM2* H1* S1* I39* I110* I27* E4* RC9* E1* H2* C9* TM1*I310* I410* RC4* RC2* I[illegible]* I210* I49* S12* TD4* I11* I46* I35

V [1]

S* P* E3* C2* TD5* S7* RC8* I36* TM2* I45* H1* H3* I110* E2* S3* E4* I16* I24*TD2* TM4* I29* I38* RC4* I46* C7* I12* I21* S8

V [1]

S* P* E3* C2* TD5* S7* RC8* I36* TM2* I45* H1* H3* I110* S3* E4* I16* I24*I29* I38* RC4*~{TM3* C1* I39* I25* I19* I47* RC9* E1}*~{TM5* S5* H4* I310*I49* TD6* C6* I13* I22}*~{I37* I44* I27* TD1* H2* S10* C9* TM1}

Concept FOR CLASS without compounds ABX_2 :

[14]

S* P* TM3*~{C1* H3}*~{RC7}*~{C2* TD5* S7* RC8* I36* TM2* I45* E4}*~{C2* H1*S1* I110* I27* E4* RC4* I46* I35}*~{E3* C5* C2* TD5* S7* RC8* I36* C1* H3*I39* RC5* I37* E5* TM5* H10* I18* TD8* S3* I25* I44* I19* I42* TD3* S6* H7*I27* I47* RC9* E1}*~{C2* TD5* S7* RC8* I36* TM2* I45* H1* S1* C1* H3* I39*RC7* I110* E2* I48* S5* I26* TD7* I27* E4* I16* I24* RC4* I46* I35}*~{C2* TD5*S7* RC8* I36* TM2* I45* H1* S1* C1* H3* I39* I110* I25* I19* I27* E4* I16*I24* I47* RC9* E1* RC4* I46* I35}*~{C2* H1* C1* H3* I39* RC7* I110* RC5* I37*E2* E5* TM5* H10* I18* I48* S5* TD8* S3* I25* I44* I26* TD7* C9* TM1* RC2*I111* I210* I49* S12}

V [14]

S* P* E3* C5*~{TM3* C2* TD5* S7* RC8* I36* C1* H3* I39* RC5* I37* E5* TM5*H10* I18* TD8* S3* I25* I44* I19* I42* TD3* S6* H7* I27* I47* RC9* E1}

V [14]

S* P* C2* TD5* S7* RC8* I36* TM2* I45*~{TM3* E4}*~{E3* H1* H3* I110* S3* E4*I16* I24* I29* I38* RC4}

V [9]

S* P* TM3* TD5* S7* C1* H3* I39*~{C2* RC8* I36* TM2* I45* I110* E4* I16* I24}*~{E3* C5* C2* RC8* I36* RC5* I37* E5* TM5* H10* I18* TD8* S3* I25* I44*

I19*I42* TD3* S6* H7* I27* I47* RC9* E1}*~{C2* RC8* I36* TM2* I45* I110* RC5* H10*I25* I26* TD7* I19* E4* I16* I24* I47* RC9* E1* TM4* I46* C3* I34* S4}*~{C2*H1* S1* E7* TD11* TM7* I110* RC5* I37* I18* I25* I44* I19* I27* E4* I47* RC9*E1* RC4* I46* I35}*~{C2* H1* S1* I110* RC5* I37* E5* TM5* H10* I18* TD8* S3*I25* I44* I19* I27* E4* I47* RC9* E1* RC4* I46* I35}*~{C2* I110* RC5* I37* E5*TM5* H10* I18* TD8* S3* I25* I44* I26* TD7* I19* E4* I47* RC9* E1* TM4* I46*C3* I34* S4}*~{S1* E7* TD11* TM7* I110* RC5* I37* H10* I18* I25* I44* I26*TD7* I19* E4* I47* RC9* E1* TM4* I46* C3* I34* S4}*~{C2* RC8* I36* TM2* I45*H1* S1* RC7* I110* E2* I48* S5* I26* TD7* I27* E4* I16* I24* RC4* I46* I35}*~{C2* RC8* I36* TM2* I45* H1* S1* I110* I25* I19* I27* E4* I16* I24* I47*RC9* E1* RC4* I46* I35}

V [5]

S* P* TM3* C2* TD5* S7* RC8* I36* TM2* I45* C1* H3* I39* I19* E4* I16* I24*I47* RC9* E1*~{I110* RC5* H10* I25* I26* TD7* TM4* I46* C3* I34* S4}*~{H1* S1*I110* I25* I27* RC4* I46* I35}

V [4]

S* P* TD5* TM2* I45* H1* I29* I38* RC4*~{E3* C2* S7* RC8* I36* H3* I110* S3*E4* I16* I24}

V [4]

S* P* TM3* E3* C2* TD5* S7* RC8* I36* TM2* I45* C1* H3* I39* I110* E4* I16*I24

V [2]

S* P* S1* C1* H3* E7* TD11* TM7*~{TM3* C2* RC8* H1* I110* RC5* I37* E2* I18*TD8* S3* I25* I44* I27* E4* I24* H4* I310* I410* I17* C4* TM4* RC4* I46* I35}*~{TM3* C2* H1* I39* RC7* I110* RC5* I37* E2* [illegible]* I48* S5* I25* I44* I26*TD7* I27* E4* RC4* I46* I35}*~{TM3* C2* TD5* S7* H1* I39* I110* RC5* I37* I18*I25* I44* I19* I27* E4* I47* RC9* E1* RC4* I46* I35}*~{TM3* TD5* S7* I39*I110* RC5* I37* H10* I18* I25* I44* I26* TD7* I19* E4* I47* RC9* E1* TM4* I46*C3* I34* S4}*~{TM3* I39* RC7* I110* RC5* I37* E2* H10* I18* I48* S5* I25* I44*I26* TD7* E4* TM4* I46* C3* I34* S4}*~{RC8* H1* I39* RC5* I37* E2* I18* TD8*S3* I25* I44* I24* C9* TM1* H4* I310* I410* I17* C4* TM4* RC2* I111* I210*I49* S12}

V [2]

S* P* C2* TD5* TM2* I45* H1* I27* C9* TM1* I29* I38* RC4

V [2]

S* P* TM3* E3* C5* C2* TD5* S7* RC8* I36* TM2* I45* C1* H3* I39* RC7* I110*E2* I48* S5* I26* TD7* E4* I16* I24

V [2]

S* P* TM3* E3* C5* C2* TD5* S7* RC8* I36* TM2* I45* H3* I110* I37* I44* I27*E4* TD1* I16* I24* H2* S10* C9* TM1

V [1]

S* P* TM3* E3* C2* TD5* S7* RC8* I36* TM2* I45* H1* C1* H3* I39* I110* S3*I25* I19* E4* I16* I24* I47* RC9* E1* I29* I38* RC4

V [1]

S* P* TM3* E3* C5* C2* RC8* I36* C1* H3* I39* RC7* I110* RC5* I37* E2* E5*TM5* H10* I18* I48* S5* TD8* S3* I25* I44* I26* TD7* I19* I42* TD3* S6* H7*I27

V [1]

S* P* TM3* E3* C5* C2* TD5* S7* RC8* I36* TM2* I45* H3* E2* TD8* S3* I44* I27*E4* I16* I24* I33* H4* TD2* I310* I410* I17* C4* TM4

V [1]

S* P* E3* C2* TD5* S7* RC8* I36* TM2* I45* H1* H3* I110* TM5* S5* S3* E4* I16*I24* H4* I310* I29* I38* RC4* I49* TD6* C6* I13* I22

V [1]

S* P* TM3* E3* C5* C2* TD5* S7* RC8* I36* TM2* I45* C1* H3* I39* RC7*
I110*RC5* E2* I48* S5* I26* TD7* E4* TD1* I28* I43* I16* I24
V [1]
S* P* TM3* E3* C5* C2* TD5* S7* RC8* I36* TM2* I45* C1* H3* I39* RC7*
I110*E2* I48* S5* I26* TD7* I19* I42* TD3* S6* H7* I27* E4* I16* I24
V [1]
S* P* E3* C2* TD5* S7* RC8* I36* TM2* I45* H1* H3* I110* I37* S3* I44*
I27*E4* TD1* I16* I24* H2* S10* C9* TM1* I29* I38* RC4

PART II

SPC-94-4097

Final Report

The Design of Inorganic Compounds: Searching for New Electro-optical, Ferro-electric, Superconducting, and Semiconducting Materials

September 1995

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Abstract

The use of computer learning strategies for predicting inorganic compounds which are believed promising as new electro-optical, ferro-electric, superconducting or semiconducting materials is explained. Prediction reliability utilizing these computer learning strategies is based on: 1) expert selection of example compounds, 2) expert assessment of data for computer learning, and 3) comparison of predictions which have been obtained using various feature sets. The classes of the inorganic compounds most promising for searching for new electro-optical, ferro-electric, superconducting, and semiconducting materials are directly based on the analysis of the application domains and known data. The results of predicting the crystal structure types at normal pressure and room temperature for the compounds with composition of AB_2Se_4 are presented. Types considered were chalcopyrite, Th_3P_4, $CaFe_2O_4$, Yb_3S_4, Yb_3Se_4, $PbGa_2Se_4$, $NiCr_2Se_4$, spinel, or olivine. Analysis of predictions showed that the structures resembling the olivine and $NiCr_2Se_4$ are an inherent feature of the compounds with composition $A(IV)B(II)_2Se_4$, but the structure types Th_3P_4 and $NiCr_2Se_4$ are characteristic of compounds with composition $A(II)B(III)_2Se_4$.

Prediction of the crystal structure types at standard conditions for the compounds with composition ABX_2 were also carried out. Types considered included chalcopyrite, alfa- or beta-$NaFeO_2$, alfa-$LiFeO_2$, or TlSe. The predictions of possibility of formation for the compounds with composition of A_3BCl_5 are presented. Analysis of results of prediction shows that few new compounds of the composition A_3BCl_5 form at normal pressure: In_3FeCl_5, Rb_3CoCl_5, and Tl_3CuCl_5. The results of predicting the crystal structure types at normal pressure and room temperature for the compounds with composition of ABF_5 are presented. Types considered were $BaFeF_5$, $BaGaF_5$, $CaFeF_5$, and $SrFeF_5$. Analysis of predictions shows: a great number of new compounds with crystal structure type $BaFeF_5$ and $CaFeF_5$, hold the promise as new electro-optical materials.

Prediction of the crystal structure types at standard conditions for the compounds with composition A_2BF_6 were also carried out. For composition $A^IB^{IV}{}_2F_6$ types considered included: Na_2SiF_6, K_2PtCl_6, K_2GeF_6-II, K_2MnF_6-II, beta-K_2UF_6, K_2ZrF_6, and tri-rutile. Analysis of results show: a great number of predictions of new compounds with crystal structure type K_2GeF_6-II and K_2ZrF_6 were obtained. New compounds with acentric space groups (crystal structure type Na_2SiF_6, space group P321): Na_2VF_6 and Na_2PaF_6, and (crystal type beta-K_2UF_6, space group P6(-)2m): Cs_2TbF_6, Tl_2TbF_6, Cs_2NpF_6, Tl_2PuF_6, K_2AmF_6, Cs_2AmF_6, Cs_2CmF_6, Tl_2CmF_6, Rb_2BkF_6, Cs_2BkF_6, Tl_2BkF_6, Rb_2CfF_6, Cs_2CfF_6, and Tl_2CfF_6, which hold the promise for searching for new electro-optical materials, were

included: Ba_2MnF_6, Ba_2CuF_6, Pb_2ZnF_6, and rutile. Analysis of results shows: a great number of predictions of new compounds with acentric crystal structure type Ba_2MnF_6 were obtained, which hold the promise for searching for new electro-optical materials.

Prediction of the crystal structure types at standard conditions for the compounds with composition $A^{II}B^{II}O_3$ and $A^{II}B^{IV}O_3$ were also carried out. Types considered included calcite, aragonite, ilmenite, $NaClO_3$, $KBrO_3$, $LiNbO_3$, and perovskite. Type of distortion (rhombic, hexagonal, monoclinic, or tetragonal) of ideal cubic perovskite cell at normal pressure and room temperature was predicted in addition. Analysis of results show that few new lithium compounds with crystal structure type $LiNbO_3$, which hold the promise for new electro-optical materials. The great number of predictions of new compounds with crystal structure type of cubic, rhombic, and monoclinic perovskite, were also obtained for compounds of composition $A^{II}B^{IV}O_3$.

An automated system for concept formation, referred to as CONFOR, was used for computer learning and prediction. The pyramidal networks and the corresponding logical expressions were formed as a result of the computer learning via CONFOR and the appendices contain those logical expressions which support the report conclusions. Certain of the logical expressions were analysed with the aim of searching for the most important combinations (conjunctions) of component property values. The search for statistical linear correlations between critical temperature of transition to superconducting state (T_c) and properties of high-temperature superconductors (HTSC) components was also carried out. Complicated perovskite-like phases were analysed: phases "1-2-3", T-, T', and T*-phases. Further information about the component properties most influencing on T_c will be used for the prediction of new HTSC and the estimation of their T_c with the help of artificial intellegence systems.

Key Words

Concept formation, computer learning, prediction, inorganic compound, electro-optical, ferro-electric, superconductor, semiconductor, chal- copyrite, spinel, perovskite, correlation, $LiNbO_3$.

FOREWORD

This report was prepared by the above identified research team under EOARD Special Contract SPC-94-4097. This is a final report summarizing research carried out over a period of twelth months from September 1994 to September 1995. This work was carried out in close contact with researchers of the Wright Laboratory - Materials Directorate. We appreciate the management leadership of Dr.Steven R.LeClair. We thank Drs. Steven R.LeClair and Allen G.Jackson for their assistance. We also acknowledge the support provided by Dr. Osama Elbayoumi, of the European Office of AFOSR, for enabling the interaction between ourselves and our colleagues from Wright Laboratory.

1. INTRODUCTION

The project's goal is to develop a new approach to a priori prediction of inorganic compounds which could be used for searching for new electro-optical, ferro-electric, superconducting or semiconducting materials with predefined properties. This approach is based on the use of computer learning strategies.

1.1. Background and Significance

The problem of calculating new multi-element compounds based on knowledge of their constituent elements properties seems to be most difficult and still remains unsolved. Calculation or prediction based on elemental properties (or simply, properties) only is called a priori calculation or prediction. The difficulties in a priori calculation arise from quantum mechanical calculations of the multi-electronic systems. An alternative to quantum mechanical calculations is the use of empirical prediction methods in which the existing regularities from a variety of property data are used. Some of these empirical criteria of the predefined properties for compound formation involving the rules of Hume-Rothery [1], Laves [2], Mathias [3], Goldschmidt [4], Villars [5], and Darken-Gurry [6].

The principle objective of finding rules is to identify linear relationships among parameter values of properties associated with constituent elements. Such rules would enable classification of physico-chemical systems into distinct domains. The appeal for such rules is simplicity and consequently the ability to depict information visibly with the help of two-dimensional plots. Often however, classification using two-dimensional plots is deficient, because other properties of the constituent elements come into play. In addition, two--dimensional rules often lose their raliability as new compound, element, and/or property data is introduced which does not easily fit within the rule boundary conditions. The ideal classification scheme must be adaptive, i.e., it must easily accommodate new examples and new property parameters, as well as have a flexible structure and be useful for recognition of any new situation. Such a classification scheme must not be limited by narrow boundaries of two-parameter planes. It is the adaptive, quick, and reliable search of these multidimensional criteria (classification rules) which motivate the following research in computer learning techniques.

1.2. Preliminary Studies

The first experiments involving "an adaptive, multidimensional" computer learning method to search for rules in the formation of the binary phases [7] have been successful. The advantage of using these computer learning methods for the multidimensional criteria search is the speed and accuracy resulting from the use of a computer to automate the task of large database analyses and the ability of the com-

puter learning method to quickly classify and re-classify a large, growing set of parameters. This computer learning method has enabled successful search for the following rules [8-13]: (1) prediction of formation (or non-formation) compound for ternary systems; (2) prediction of the possibility of forming ternary and more complicated compounds of desired composition; (3) prediction of phases with definite crystal structures; (4) estimation of phase quantitative properties (critical temperature of transition to superconducting state, homogeneity region, etc.).

The computer learning method we employ is based upon a cybernetic approach referred to as "pyramidal-nets" wherein we have predicted the formation of thousands of new compounds in ternary, quaternary and more complicated systems. These compounds were searched to identify new semiconductors, superconductors, ferro-electrics, magnets, and other materials required for new technology [8-13]. The comparison of these predictions with the experimental data established [8] an average reliability of the predicted ternary phases exceeding 80 % - a higher a priori prediction accuracy than by any theoretical method known.

1.3. Research Design and Methods

In principle there are three ways to predict new electro-optical, ferro-electric, superconducting, and semiconducting inorganic compounds based upon knowledge of their constituent element properties to forecast the intrinsic compound properties:

- quantum-mechanical calculations;
- two-dimensional criteria (classification rules) found by different semi-empirical approaches;
- computer learning methods (cybernetic prediction).

As stated above the cybernetic approach seems to be more suitable for a priori prediction of the inorganic substances.

1.4. Methods of Prediction

As a precursor to the cybernetic approach [14] referenced above, multidimensional cybernetic prediction of inorganic compounds was originally applied by Mendeleev to establish that the periodic change in the properties of chemical systems depends on the properties and nature of the elements which form these systems (compounds, solutions and so on).

Our cybernetic approach has enabled us to reduce the problem of "new--compound" prediction to the analysis of a multidimensional array of property values and the column vector of the desired property. Each row corresponds to some already known physical-chemical system, i.e., a compound, whose class membership is a priori decided by the researcher. The process of analysing this infomation is aimed at finding

regularities or boundaries associated with those compounds within the class. These boundaries are used subsequently to establish whether a new, yet to be evaluated, compound is indeed a member of the class of interest. By substituting the property values of this new compound in the regularity (class boundaries) thus found, it becomes possible to predict the class membership of the new compound. The implementation of this stage (called the "prediction") requires only the knowledge of the values of the component properties.

After testing many methods intended for computer learning applications, we selected an algorithm referred to as Gladun's Algorithm in which all classifying regularities could be presented in the form of a Boolean expression or an equivalent semantic network [14]. We have used this approach on databases of properties of ternary inorganic compounds and on the properties of the crystals of acousto-optical, electro-optical, and nonlinear-optical materials to predict new inorganic phases with predefined composition and crystal type which are similar to known electro-optical, ferro-electric, superconducting, magnet, or semiconducting compounds in this research.

2. APPLICATION OF COMPUTER LEARNING METHODS

2.1.Definitions

Physical-chemical system. - is a system (e.g., compound, or solid solution) which is formed from chemical elements.

Object. - is a physical-chemical system which is described as a set of property (feature) values of the constituent elements.

Feature. - is a property of the constituent component of the physical--chemical system.

Learning set. - is a multidimensional array of feature values and a column vector of the desired property. Each row corresponds to some physical-chemical system already known, whose class is indicated by row position of the column vector.

Set for prediction. - is a multidimensional array of feature values. Each row corresponds to some unknown physical-chemical system, whose class is necessary to predict.

Qualitative property. - is an object or element property which can be described as a qualitative concept (e.g., multi-element system with compound formation or non-formation, crystal structure type, possibility of forming compounds of desired composition, and so on).

uantitative property. - is an object or element property which has a numeric values from some continuum (quasi-continuum) set of numbers (e.g., melting point, birefringence, index of refraction, and so on).

Note: There are two preparatory steps in using computer learning methods:

1) selection of a learning set of compounds which a priori have been determined to be within the class of interest and those to be outside of the class of interest;

2) selection of the relevant properties (features) of the constituent elements of those compounds upon which the class boundary will be established.

A problem of selection of the threshold values for the classification arises during the attempt of estimation of unknown quantitative properties (e.g., melting point of compounds). This last problem is similar to the problem of quantization (discretization) of continuous quantitative constituent component properties arising with the use of logical algorithms of computer learning, including Gladun's Algorithm [14].

2.2.Selection of Examples for Computer Learning

The computer learning is carried out on examples of known physical--chemical systems with an a priori determination of their belonging to a certain class. If the number of examples in the learning set is not enough and/or examples are not representative of the class of interest, then the resulting classification by regularity describes only that small region of the multidimensional space in which these objects reside. In this case, use of the classification rules for prediction will be unsuccessful. The number and representativeness of the learning set increases if the prediction (estimation) of some unknown quantitative property is desired, e.g., values of birefringence for a chalcopyrite require hundreds of examples in order to obtain acceptable results. Learning set examples which were classified incorrectly introduce large error into the prediction reliability. More specifically, all analogs of the incorrectly classified example will be recognized erroneously. Thus, expert assessment of the examples for the learning set is most important.

2.3. Selection of the Properties (Features)

The number of element properties (i.e., elements and/or simple compounds) required for compound classification has been much studied extensively and is considered to be less than 100. Our research suggests that more important than the number of properties is the selection of properties (herein referred to as features). The selection of those properties which are most representative of the class of interest is the most important consideration for materials scientist.

Gladun's Algorithm of computer learning [14] allows us to reject those property values which have no importance for the classification process, i.e., those properties which do not appear in a rule are not relevant. Thus, it is desirable that the concept formation aspect of Gladun's Algorithm be exercised using a reasonable set of properties. Upon exercise of concept formation those properties which are not relevant can be eliminated from further evaluation. It is necessary to

restrict the initial set of properties to a reasonable number on the basis of theoretical physical and chemical grounds by means of expert assessment. An important feature of Gladun's Algorithm [14] which is beneficial for predicting inorganic compound properties is the ability to exercise the algorithm with incomplete property information or ranges where no information exists. It should be noted that if the "gaps" of information regarding a property exceeds 10%, this property should not be selected for classification.

2.4.Selection of Threshold Values for Classification

The problem of computer learning is simplified if the concept or rule sought is formed about a well known class of substances (e.g., the class of physical-chemical systems with elements from a certain composition or definite crystal structure type as chalcopyrite, perovskite and the like). Clearly all these concepts are "fuzzy", because it is difficult to establish a definite boundary (threshold value) for the concept of interest.

This fuzziness is characterized by the difficulty of establishing a boundary between similar compounds when processing conditions are unknown, e.g., distinguishing a pure stoichiometric compound and a non-stoichiometric compound (i.e., with wide homogeneity range in terms of composition) or between spatially varying crystal structures such as an orthorhombically or a tetragonally distorted perovskite and a classic cubic perovskite. Variations in processing conditions, specimen preparation and/or property measurement lead to uncertainty in property data which is unresolved even by qualified experts. In addition, the vagueness of any concept used by a researcher is a source of further inaccuracy of prediction based on computer learning using the learning set.

The problem becomes even more complicated if it is necessary to predict some quantitative property (e.g., the melting point or birefringence of a compound). The hypothesis of class compactness, based on methods of computer learning presupposes that the different classes locate compactly in the multidimensional feature space and there are not intersections between these classes. But we found such a set of properties whose space contradict this hypothesis. The application of cluster analysis to the example learning set in combination with the grouping of features according to statistical correlation allows us to decrease the intersections of classes, but only slightly, owing to the selection of the natural (for certain learning set) threshold values of predicted quantitative property. Note these natural threshold value are less a consequence of the nature of phases and more the set of examples for the computer learning method. These observations are based upon the learning set examples which have been obtained and investigated at present.

Therefore, as a consequence of the above interaction problem, the attempt to predict certain threshold values which are important for technological applications, e.g., boiling point temperatures of helium and nitrogen for superconducting compounds, is justified only from a

practical standpoint. The error of this prediction will be high, but it will be possible to predict (with high reliability) those objects which are widely spaced in the features space. A priori identification of these objects by a researcher seems to be a great problem. One possibility to solve this problem is to visualize a two-dimensional projection of points, which corresponds to the objects of the learning set, in combination with cluster analysis of objects and grouping features according to statistical correlation. The algorithms for this system involve cluster analysis based on the method of potential functions [15,16] and the extreme grouping of parameters [16]. Both have been applied manually, but implementation for automated use will require more than two manyears of efforts.

As stated above, prediction accuracy of quantitative properties depends strongly on the volume and representativeness of the learning set. Our experience shows that the number of the learning examples must equal 100s or even 1000s in order to have acceptable estimation of quantitative property.

2.5.Quantization (Discretization) of Continuous Constituent Element Properties

The problem of quantization is a peculiarity of the logical algorithms of the computer learning method. This problem is closely related to the last-mentioned problem of the selection of the threshold values for the computer classification. Quantization is easy to solve if the classification has a qualitative nature (in case of the prediction of qualitative properties). For examlpe, the types of the incomplete electronic shells have four gradation: s-, p-, d-, and f--shell. In the simplest cases, if quantitative properties are integer numbers in the narrow range, it makes sense to assign its gradation to each property value. For example, the number of electrons of the s-shell of the isolated atoms has three gradations: 0, 1 and 2; the formal valency of the element in ionic compounds has eight gradations: 1, 2, 3, 4, 5, 6, 7, and 8.

The problem with the selection of the number of gradations is that they are purely empirical and somewhat arbitrary. It is important to consider that the increase in the number of gradations leads to the decrease in our ability to generalize about the properties of a concept and therein will necessitate an increase of the number of examples in the learning set. At the same time it is obvious that too small a number of gradations leads to the intersection of classes.

It would be ideal if the boundaries between the different feature gradations separate one class of the learning set from another. This idea of solution of the inverse task is a basis of the algorithm of feature quantization which was developed in [17]. At a later time it makes sense to supply the program system of concept formation CONFOR [14] with the programs of the feature preprocessing based on this algorithm [17].

2.6.Ways of Improving the Reliability of Predicting

2.6.1. Utilization of Databases for the Selection of the "Learning Step" Examples

The developed database [18-21] containing ternary compound properties is used for the search information for the computer learning. Our database [20-23] containing the information about the compounds which possess acousto-optical, electro-optical and non-linear optical properties will be used for the search information for the estimation of the properties of substances of this kind. The data about quaternary compounds will be extracted from our card file containing information about the properties of compounds which contain four chemical elements.

2.6.2. Expert Assessment of Data

This is the most difficult problem for the expert who teaches the computer.

2.6.3. Comparison of Predictions Which Have Been Obtained Using Various Property (Feature) Sets

All the properties of chemical elements and compounds are correlated to one another, because they all depend on atomic numbers of elements or combinations of elements (for compounds). In this connection the predictions which have been obtained using different feature sets must be consistent. Lack of consistency is caused by poor quantization of property values and, consequently, by the "fuzzy" boundaries of the concepts which have been formed from the learning set examples. Further, inaccuracy of measurement of the element properties contributes to this fuzziness. However, in individual cases, the lack of consistency may indicate that the learning set examples exhibit a limited set of classes (e.g., the compound has few polymorphous crystal modifications within narrow limits of temperature and pressure).

If the results of prediction, using the different feature sets, contradict one another in the process of the comparison, then the predictions will be rejected in the resulting table, i.e., if the result of prediction using the first feature set is positive, but the result using the second feature set is negative, then the resulting prediction is rejected, and the empty square corresponds to an inconsistency in the resulting table of predictions. When the result of a prediction using the second feature set is vague (designated by an "X" in the table) then it is assumed that the prediction using the first feature set is a true one, i.e. the positive prediction is included in the resulting table.

3. SELECTION OF INORGANIC COMPOUNDS FOR PREDICTION OF NEW ELECTRO-OPTICAL, FERRO-ELECTRIC, SUPERCONDUCTING AND SEMICONDUCTING MATERIALS

3.1. Promising Phases for Searching for New Ferro-Electric and Electro-Optical Materials

Composition	Crystal structure type	Space group	Examples	Applications	Reference #
ABO_3	Distorted ilmenite	acentric groups	$LiNbO_3$ $LiTaO_3$	Electro-optical materials	24
ABO_3	Distorted perovskite	acentric groups	$PbTiO_3$ $BaTiO_3$ $PbZrO_3$ $SrTiO_3$	Electro-optical materials	24
A_2BCHal_6	Elpasolith	Fm3m	K_2LiGaF_6	Laser matrix	24
AB_2Chal_4	Th_3P_4	I4(-)3d	-	Electro-optical materials	24
ABX_2 AB_2X_4	Chalcopyrite	I4(-)2d	$ZnGeP_2$ $CdGa_2S_4$	Electro-optical materials	24
A_2BF_6	-	acentric groups	Ba_2ZnF_6 Sr_2CuF_6	Electro-optical materials	24
ABX	PbFCl	P4/nmm	PbFCl	Polarization optics	24
A_3BCl_5	-	acentric groups	Tl_3PbCl_5	IR-elecro-acousto-optics	24
ABF_5	-	acentric groups	$SrAlF_5$	Laser matrix	24
$A_2BC_2O_7$	Melilite	P4(-)2 m_1	$Ba_2ZnGe_2O_7$ $Ba_2MgGe_2O_7$	Laser matrix	24

3.2. Promising Phases for Searching for New Semiconductors and Magnet Semiconductors

Composition	Crystal structure type	Space group	Examples	Applications	Reference #
AB_2Se_4	Spinel	Fd3m	$CdCr_2Se_4$	Data storage and processing devices, magneto-optics, non-linear capacitors, microwave integrated circuits, and so on	25

3.3. Phases Which Hold the Promise for Searching for New Superconductors

Composition	Crystal structure type	Space group	Examples	Applications	Reference #
$R_x R'_{2-x} CuO_4$	T'		$Nd_x Ce_{2-x} CuO_4$	Electron-doped high temperature superconductors	26,27
AB_2Chal_4	Spinel	Fd3m	$CuRh_2Se_4$ $CuRh_2S_4$ CuV_2S_4	Superconductors	32

3.4. Predicting New Compounds of Composition AB_2Se_4 with Crystal Structure Types of Th_3P_4, Chalcopyrite, Spinel, and etc.

Phases with crystal type Th_3P_4 (space group I4(-)3d) [29,31] are of interest for compounds which hold promise for new semiconducting and electro-optical materials [24,25]. We attempted to predict the new chalcopyrites (space group I4(-)2d) [28,29] of composition AB_2Se_4 (the examples of promised compound $CdGa_2S_4$ with interesting electro-optical properties) [24].

In searching for new semiconductors, superconductors, and magnet semiconductors, we attempted to predict new selenides of composition AB_2Se_4 and spinel crystal structure type (space group Fd3m) [25,29, 31-34]. These compounds are of interest for development of data storage and processing devices, magneto-optics, non-linear capacitors, microwave integrated circuits, and so on [25].

3.4.1. Data for Computer Learning

The data for computer learning was extracted from the DB on ternary inorganic compound properties [18-21]. We had predicted the new selenides of this composition and with structure types of spinel [8,36], Th_3P_4, $CaFe_2O_4$, and $NiCr_2Se_4$ previously [8]. In this investigation all information for the computer learning was assessed by expert on the inorganic compounds of selenium Dr.T.I.Koneshova (Kurnakov Institute of General and Inorganic Chemistry of RAN). Table 3.4.1 contains a resulting learning set.

Table 3.4.1
Learning set for Predicting Crystal Types with Composition AB_2Se_4

Composition	Crystal type
GeHg2Se4	chalcopyrite
ZnAl2Se4	chalcopyrite
CdAl2Se4	chalcopyrite
ZnGa2Se4	chalcopyrite
ZnIn2Se4	chalcopyrite
CdGa2Se4	chalcopyrite
HgGa2Se4	chalcopyrite
CdIn2Se4	chalcopyrite
HgIn2Se4	chalcopyrite
SnMg2Se4	olivin
SiCa2Se4	olivin
SiMn2Se4	olivin
VTi2Se4	NiCr2Se4
CoSi2Se4	NiCr2Se4
NiSi2Se4	NiCr2Se4
TiCr2Se4	NiCr2Se4
CrTi2Se4	NiCr2Se4

Composition	Crystal type
MnTi2Se4	NiCr2Se4
TiFe2Se4	NiCr2Se4
FeTi2Se4	NiCr2Se4
CoTi2Se4	NiCr2Se4
NiTi2Se4	NiCr2Se4
MnV2Se4	NiCr2Se4
VFe2Se4	NiCr2Se4
FeV2Se4	NiCr2Se4
NiV2Se4	NiCr2Se4
NiCr2Se4	NiCr2Se4
TiTi2Se4	NiCr2Se4
VV2Se4	NiCr2Se4
CrCr2Se4	NiCr2Se4
FeFe2Se4	NiCr2Se4
CrRh2Se4	NiCr2Se4
CoRh2Se4	NiCr2Se4
NiRh2Se4	NiCr2Se4
FeGa2Se4	spinel
MnSc2Se4	spinel
CuCr2Se4	spinel
ZnCr2Se4	spinel
CdCr2Se4	spinel
HgCr2Se4	spinel
CuMn2Se4	spinel
ZnMn2Se4	spinel
CuRh2Se4	spinel
CdY2Se4	spinel
CdDy2Se4	spinel
CdHo2Se4	spinel
CdEr2Se4	spinel
CdTm2Se4	spinel
CdYb2Se4	spinel
CdLu2Se4	spinel
SrAl2Se4	PbGa2Se4
EuAl2Se4	PbGa2Se4
YbAl2Se4	PbGa2Se4
PbAl2Se4	PbGa2Se4
CaGa2Se4	PbGa2Se4
SrGa2Se4	PbGa2Se4
BaGa2Se4	PbGa2Se4
EuGa2Se4	PbGa2Se4
YbGa2Se4	PbGa2Se4
PbGa2Se4	PbGa2Se4
SmIn2Se4	PbGa2Se4
EuIn2Se4	PbGa2Se4
YbIn2Se4	PbGa2Se4
CrLa2Se4	Th3P4
CrCe2Se4	Th3P4

Composition	Crystal type
CrPr2Se4	Th3P4
CrNd2Se4	Th3P4
CrSm2Se4	Th3P4
CrEu2Se4	Th3P4
PbLa2Se4	Th3P4
PbCe2Se4	Th3P4
PbPr2Se4	Th3P4
PbNd2Se4	Th3P4
PbSm2Se4	Th3P4
SmNd2Se4	Th3P4
SmSm2Se4	Th3P4
CdLa2Se4	Th3P4
CdPr2Se4	Th3P4
CdGd2Se4	Th3P4
EuLa2Se4	Th3P4
EuCe2Se4	Th3P4
EuPr2Se4	Th3P4
EuNd2Se4	Th3P4
EuSm2Se4	Th3P4
EuGd2Se4	Th3P4
EuTb2Se4	Th3P4
CeCe2Se4	Th3P4
PrPr2Se4	Th3P4
NdNd2Se4	Th3P4
ULa2Se4	Th3P4
UCe2Se4	Th3P4
UPr2Se4	Th3P4
UNd2Se4	Th3P4
USm2Se4	Th3P4
UGd2Se4	Th3P4
UU2Se4	Th3P4
NpNp2Se4	Th3P4
PuPu2Se4	Th3P4
AmAm2Se4	Th3P4
CaY2Se4	Yb3S4
CaHo2Se4	Yb3S4
YbHo2Se4	Yb3S4
YbEr2Se4	Yb3S4
YbTm2Se4	Yb3S4
CaDy2Se4	Yb3Se4
CaEr2Se4	Yb3Se4
CaYb2Se4	Yb3Se4
CaLu2Se4	Yb3Se4
YbYb2Se4	Yb3Se4
EuSc2Se4	CaFe2O4
SrY2Se4	CaFe2O4
SrTb2Se4	CaFe2O4

Composition	Crystal type
SrDy2Se4	CaFe2O4
SrHo2Se4	CaFe2O4
SrEr2Se4	CaFe2O4
SrTm2Se4	CaFe2O4
SrYb2Se4	CaFe2O4
SrLu2Se4	CaFe2O4
BaY2Se4	CaFe2O4
BaSm2Se4	CaFe2O4
BaGd2Se4	CaFe2O4
BaDy2Se4	CaFe2O4
BaYb2Se4	CaFe2O4
BaLu2Se4	CaFe2O4
EuHo2Se4	CaFe2O4
EuEr2Se4	CaFe2O4
EuTm2Se4	CaFe2O4
EuYb2Se4	CaFe2O4
EuLu2Se4	CaFe2O4
PbEr2Se4	CaFe2O4
PbTm2Se4	CaFe2O4
PbYb2Se4	CaFe2O4
PbLu2Se4	CaFe2O4

Composition	Crystal type	Space group	Z
SiBa2Se4	GeSr2S4	P2(1)/m	2
FeSi2Se4	CdI2		
GeZn2Se4	ZnS		
GeCd2Se4	GeCd2S4	rhombohedric	9
GeEu2Se4	GeSr2S4	P2(1)/m	2
GeYb2Se4	GeSr2S4	P2(1)/m	2
SnHg2Se4		I4(-)	
MgAl2Se4		R3m	
MgIn2Se4		R3m	
BaAl2Se4		P4/nnc	4
CaIn2Se4		P2(1)2(1)2(1)	4
SrV2Se4		hexagonal	
EuV2Se4		hexagonal	9
SrCr2Se4		hexagonal	
BaCr2Se4		hexagonal	
EuCr2Se4	PbCr2S4	P6	9
CrTb2Se4		rhombic	12
CrDy2Se4		rhombic	12
CrLu2Se4		rhombic	12
PbCr2Se4		hexagonal	
MnGa2Se4		ZnS	
MnAs2Se4		tetragonal	2
MnBi2Se4		tetragonal	
CdTl2Se4		hexagonal	
SnSb2Se4		Pnnm	12
SnNd2Se4		Fdd2	16
BaSb2Se4		P2(1)/n	8
EuSb2Se4	PbBi2S4	P2(1)2(1)2(1)	
BaBi2Se4		P6(3)/m	12
CuGa2Se4	ZnS		

Pseudo-Binary Systems with Se anions in which AB_2Se_4 is not formed

ZnSe-SnSe2	without	compound	AB2Se4
GaSe-GeSe2	without	compound	AB2Se4
InSe-GeSe2	without	compound	AB2Se4
SnSe-GeSe2	without	compound	AB2Se4
CdSe-SnSe2	without	compound	AB2Se4
TlSe-SnSe2	without	compound	AB2Se4
SnSe2-AuSe	without	compound	AB2Se4
SnSe2-InSe	without	compound	AB2Se4
USe-Sc2Se3	without	compound	AB2Se4
USe-Ho2Se3	without	compound	AB2Se4
USe-Er2Se3	without	compound	AB2Se4
USe-Tm2Se3	without	compound	AB2Se4

USe-Lu2Se3 without compound AB2Se4
USe-Y2Se3 without compound AB2Se4
GaSe-As2Se3 without compound AB2Se4
CuSe-Nd2Se3 without compound AB2Se4
CuSe-Gd2Se3 without compound AB2Se4
SmSe-As2Se3 without compound AB2Se4
YbSe-Ce2Se3 without compound AB2Se4
YbSe-Pr2Se3 without compound AB2Se4
YbSe-Nd2Se3 without compound AB2Se4
YbSe-Eu2Se3 without compound AB2Se4
YbSe-Gd2Se3 without compound AB2Se4
YbSe-Tb2Se3 without compound AB2Se4
YbSe-Dy2Se3 without compound AB2Se4
SnSe-Ga2Se3 without compound AB2Se4
CdSe-Sn2Se3 without compound AB2Se4
TlSe-Ga2Se3 without compound AB2Se4
GaSe-Tl2Se3 without compound AB2Se4
GeSe-Sb2Se3 without compound AB2Se4
CdSe-As2Se3 without compound AB2Se4
NdSe-As2Se3 without compound AB2Se4
HgSe-As2Se3 without compound AB2Se4
SnSe-In2Se3 without compound AB2Se4
SnSe-Au2Se3 without compound AB2Se4
SnSe-Bi2Se3 without compound AB2Se4
HgSe-Sb2Se3 without compound AB2Se4
HgSe-Bi2Se3 without compound AB2Se4
CrSe-In2Se3 without compound AB2Se4
CoSe-In2Se3 without compound AB2Se4
CuSe-In2Se3 without compound AB2Se4
ZnSe-Bi2Se3 without compound AB2Se4
GeSe-Ga2Se3 without compound AB2Se4
GeSe-In2Se3 without compound AB2Se4

At first we predicted the possibility of forming compounds of composition AB_2Se_4 (divided into two classes - dichotomy). Next, we predicted the crystal types (chalcopyrite [28,29], spinel [25,29,31-34], Th_3P_4 [24,25,31], $PbGa_2Se_4$ (space group Cccm) [30], Yb_3S_4 (space group $Cmc2_1$), Yb_3Se_4 (rhombohedral structure), $CaFe_2O_4$ (space group Pnam), $NiCr_2Se_4$ (space group $C2/m$), and olivin (space group Pbnm)) at standard conditions (at room temperature and normal pressure) for predicted on the first stage compounds (multiclass predicting).

3.4.2. Selection of Features

On the basis of physical-chemical grounds three sets of constituent component features were selected for the description of selenide systems and compounds.

3.4.2.1. Feature Set I

Set I includes information about the number of electrons in energy shells of separate atoms, the covalent radii, and the formal valence of elements A or B in the compound of composition AB_2Se_4. The grouping of energy shell information (hereafter referred to as gradation) corresponds to the number of electrons for each shell and their respective valence value. The quasi-continuous property - the covalent radius - was divided (quantized) on the basis of the uniform distribution of the values of the intervals. Table 3.4.2 contains the gradations for Feature Set I.

Table 3.4.2
Gradations for Feature Set I

Feature	Gradation	Feature	Gradation
1s-shell		5d-shell	
s1	S11	d0	D50
s2	S12	d1	D51
2s-shell		d2	D52
s0	S20	d3	D53
s1	S21	d4	D54
s2	S22	d5	D55
2p-shell		d6	D56
p0	P20	d7	D57
p1	P21	d9	D59
p2	P22	d10	D510
p3	P23	5f-shell	
p4	P24	f0	F50
p5	P25	f2	F52
p6	P26	f3	F53
3s-shell		f4	F54
s0	S30	f5	F55
s1	S31	f6	F56

Feature	Gradation	Feature	Gradation
s2	S32	f7	F57
3p-shell		f8	F58
p0	P30	f10	F510
p1	P31	f11	F511
p2	P32	f12	F512
p3	P33	f13	F513
p4	P34	f14	F514
p5	P35	6s-shell	
p6	P36	s0	S60
3d-shell		s1	S61
d0	D30	s2	S62
d1	D31	6p-shell	
d2	D32	p0	P60
d3	D33	p1	P61
d4	D34	p2	P62
d5	D35	p3	P63
d6	D36	p4	P64
d7	D37	p5	P65
d8	D38	p6	P66
d10	D310	6d-shell	
4s-shell		d0	D60
s0	S40	d1	D61
s1	S41	d2	D62
s2	S42	7s-shell	
4p-shell		s0	S70
p0	P40	s1	S71
p1	P41	s2	S72
p2	P42	Valency	
p3	P43	+1	B1
p4	P44	+2	B2
p5	P45	+3	B3
p6	P46	+4	B4
4d-shell		+5	B5
d0	D40	+6	B6
d1	D41	+7	B7
d2	D42	+8	B8
d3	D43	Covalent or	
d4	D44	metallic	
d5	D45	radius, A	
d6	D46	[0.028-1.04]	R1
d7	D47	(1.04-1.3]	R2
d8	D48	(1.3-1.36]	R3
d10	D410	(1.36-1.43]	R4
4f-shell		(1.43-1.58]	R5
f0	F40	(1.58-1.62]	R6
f2	F42	(1.62-1.75]	R7
f3	F43	(1.75-1.82]	R8
f4	F44	(1.82-1.88]	R9

Feature	Gradation	Feature	Gradation
f5	F45	(1.88-2.80]	R10
f6	F46		
f7	F47		
f8	F48		
f10	F410		
f11	F411		
f12	F412		
f13	F413		
f14	F414		
5s-shell			
s0	S50		
s1	S51		
s2	S52		
5p-shell			
p0	P50		
p1	P51		
p2	P52		
p3	P53		
p4	P54		
p5	P55		
p6	P56		

3.4.2.2 Feature Set II

Set II includes the following information: the first three ionization potentials, the electronegatives, the types of incomplete electronic shells, the number of electrons in the incomplete electronic shell, the covalent or metallic radii, the ratio of the atomic number to the average atomic mass for atoms of elements A and B, the standard enthalpies of formation of corresponding simple selenides, the number of the group in Periodic Table and the formal valences exhibited in an AB_2Se_4 compound. The quantitative properties (ionization potentials, the electronegatives, the covalent or metallic radii, the standard enthalpies of formation) were quantized on the basis of the uniform distribution of the values of the intervals. Table 3.4.3 contains the gradations for Feature Set II.

Table 3.4.3
Gradations for Feature Set II

Feature	Gradation	Feature	Gradation
Type of incomplete electronic shell		Ratio of the atomic number to the average atomic mass,	
s	S	1/c.u.	NM1
p	P	0.99	NM2
d	D	0.50	NM3
f	F	0.49	NM4
Electronegative		0.48	NM5
[0.7-1]	Ne1	0.47	NM6
(1-1.2]	Ne2	0.46	NM7
(1.2-1.3]	Ne3	0.45	NM8
(1.3-1.6]	Ne4	0.44	NM9
(1.6-1.8]	Ne5	0.43	NM10
(1.8-1.9]	Ne6	0.42	NM11
(1.9-2.1]	Ne7	0.41	NM12
(2.1-2.2]	Ne8	0.40	NM13
(2.2-4]	Ne9	0.39	
First ionization potential, eV		Number of of electrons in the incomplete electronic shell	
[3.893-5.39]	I11		
(5.39-5.90]	I12		
(5.90-6.31]	I13		
(6.31-6.74]	I14	0	E0
(6.74-6.95]	I15	1	E1
(6.95-7.432]	I16	2	E2
(7.432-7.87]	I17	3	E3
(7.87-8.64]	I18	4	E4
(8.64-9.30]	I19	5	E5
(9.30-10.55]	I110	6	E6
(10.55-25]	I111	7	E7
Second ionization potential, eV		8	E8
		9	E9
		10	E10
[0-11.5]	I21	11	E11
(11.5-12.4]	I22	12	E12
(12.4-14.2]	I23	13	E13
(14.2-15.92]	I24	Number of of group	
(15.92-16.904]	I25		
(16.904-18.7]	I26	1	N1

Feature	Gradation	Feature	Gradation
(18.7-19.65]	I27	2	N2
(19.65-21.5]	I28	3	N3
(21.5-27.56]	I29	4	N4
(27.56-75.62]	I210	5	N5
Third		6	N6
ionization		7	N7
potential, eV		8	N8
[0-21]	I31	Standard	
(21-24]	I32	enthalpy of	
(24-25.61]	I33	formation for	
(25.61-29]	I34	corresponding	
(29-30.64]	I35	simple	
(30.64-32.8]	I36	selenide,	
(32.8-34.21]	I37	kcal/mol	
(34.21-37]	I38	[-66 - -12.2]	H1
(37-47.426]	I39	(-12.2 - -8]	H2
(47.426-154]	I310	(-8 - 0]	H3
Covalent or		(0 - 14]	H4
metallic		(14 - 18]	H5
radius, A		(18 - 24.5]	H6
[0.28-1.04]	R1	(24.5 - 36.64]	H7
(1.04-1.21]	R2	(36.64 - 50.8]	H8
(1.21-1.25]	R3	(50.8 - 82]	H9
(1.25-1.26]	R4	(82 - 223]	H10
(1.26-1.27]	R5	Formal	
(1.27-1.30]	R6	valency	
(1.30-1.34]	R7	1	Se21
(1.34-1.37]	R8	2	Se11
(1.37-1.38]	R9	3	Se23
(1.38-1.40]	R10	4	Se12
(1.40-1.44]	R11	5	Se13
(1.44-1.54]	R12		
(1.54-1.75]	R13		
(1.75-1.82]	R14		
(1.82-1.83]	R15		
(1.83-1.87]	R16		
(1.87-2.8]	R17		

3.4.2.3 Feature Set III

Feature set III includes the following information: the covalent or metallic radii for the elements A and B, the standard enthalpies of

formation of corresponding simple selenides, and the standard entropies of simple selenides. These quantitative properties were quantized on the basis of uniform distribution of the values of the intervals. Table 3.4.4 contains the gradations for Feature Set III.

Table 3.4.4
Gradations for Feature Set III

Feature	Gradation	Feature	Gradation
Type of incomplete electronic shell		Standard enthalpy of formation for corresponding simple selenide, kcal/mol	
s	S		
p	P		
d	D		
f	F		
Electronegative		[-66 - -12.2]	H1
		(-12.2 - -8]	H2
[0.7-1]	Ne1	(-8 - 0]	H3
(1-1.2]	Ne2	(0 - 14]	H4
(1.2-1.3]	Ne3	(14 - 18]	H5
(1.3-1.6]	Ne4	(18 - 24.5]	H6
(1.6-1.8]	Ne5	(24.5 - 36.64]	H7
(1.8-1.9]	Ne6	(36.64 - 50.8]	H8
(1.9-2.1]	Ne7	(50.8 - 82]	H9
(2.1-2.2]	Ne8	(82 - 223]	H10
(2.2-4]	Ne9	Standard entropy for corresponding simple selenide, cal/mol*K	
Covalent or metallic radius, A			
[0.28-1.21]	R1		
(1.21-1.26]	R2		
(1.26-1.30]	R3	[1-15.7]	S1
(1.30-1.37]	R4	(15.7-18]	S2
(1.37-1.40]	R5	(18-19.2]	S3
(1.40-1.54]	R6	(19.2-20.74]	S4
(1.54-1.82]	R7	(20.74-22.5]	S5
(1.82-1.87]	R8	(22.5-24.5]	S6
(1.87-2.8]	R9	(24.5-26.9]	S7
Formal valency		(26.9-39]	S8
		(39-53.2]	S9
0	B0	(53.2-96]	S10
1	B1		
2	B2		
3	B3		
4	B4		
5	B5		
6	B6		
7	B7		
8	B8		

3.4.3. Prediction of Formation

In the case of predicting the formation of the compounds with composition AB_2Se_4 the computer learning is carried out for three learning sets in which the compounds from Table 3.4.1 were described in terms of the sets of the component properties I-III. The system of concept formation CONFOR [14] was used for computer learning and prediction.

Since computer memory capacity for the storage of semantic networks for the learning sets in the terms of I and II became more then 65,500 symbols, the corresponding learning sets were divided into two sets: for the compounds of formally two- and four-valence elements and for the compounds of formally two- and three-valence elements.

3.4.4. Prediction of Crystal Structure

In the case of predicting the crystal structure type of the compounds with composition AB_2Se_4 computer learning is carried out for three learning sets in which the compounds from Table 3.4.1 were described in terms of the sets of the component features I-III. The system of concept formation, CONFOR, [14] was used for computer learning and predicting.

Again, the problem of computer memory capacity for storage of semantic net for the learning sets in the terms of I and II arises, the learning process was divided into two stages: for the compounds of formally two- and four-valence elements and for the compounds of formally two- and three-valence elements.

The pyramidal networks and the corresponding logical expressions were formed as a result of the computer learning via CONFOR. Appendix 1 contains the logical expressions for various learning sets. Hereafter, the following conventional signs were used: V - a disjunction sign, * - a conjunction sign, and *~, or *-, or -* - a negation sign. The number in square brackets is the number of iterations of a fragment of the logical expression in a learning set.

3.4.5. Description in terms of Feature Set I

In the case of the descriptions in terms of feature set I, some of the objects from Table 3.4.1 were selected for the examination. The results of examination testify (Table 3.4.5) that there is a vagueness of recognition which suggests that the level of the computer training, in the case of the description in terms of the distribution of electrons in the shells of separate atoms, the covalent radii, and the corresponding formal valence, is rather bad (Table 3.4.6).

Table 3.4.5
Set for Examination

Composition	Crystal type	Result of examination
CdAl2Se4	chalcopyrite	X
ZnGa2Se4	chalcopyrite	X
CdCr2Se4	spinel	X
CdHo2Se4	spinel	X
CdEr2Se4	spinel	X
SrGa2Se4	PbGa2Se4	X
YbGa2Se4	PbGa2Se4	X
CrTi2Se4	NiCr2Se4	NiCr2Se4
CoTi2Se4	NiCr2Se4	X
CrPr2Se4	Th3P4	X
PbNd2Se4	Th3P4	X
CdPr2Se4	Th3P4	X
EuCe2Se4	Th3P4	X
EuGd2Se4	Th3P4	X
YbTm2Se4	Yb3S4	Yb3S4
CaEr2Se4	Yb3Se4	X
SrDy2Se4	CaFe2O4	X
SrYb2Se4	CaFe2O4	X
BaGd2Se4	CaFe2O4	X
BaYb2Se4	CaFe2O4	X
PbTm2Se4	CaFe2O4	X
CrDy2Se4	another structure	X
YbSe-Pr2Se3	without AB2Se4	without AB2Se4
YbSe-Sm2Se3	without AB2Se4	X
YbSe-Dy2Se3	without AB2Se4	without AB2Se4

Table 3.4.6
ESTIMATION OF RESULTS OF EXAMINATION

Class of chalcopyrite :
number of objects - 2 ;
correctly - 0 [0 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 2 [100 %] ;

Class of spinel :
number of objects - 3 ;
correctly - 0 [0 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 3 [100 %] ;

Class of PbGa2Se4 :
number of objects - 2 ;
correctly - 0 [0 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 2 [100 %] ;

Class of NiCr2Se4 :
number of objects - 2 ;
correctly - 1 [50 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 1 [50 %] ;

Class of Th3P4 :
number of objects - 5 ;
correctly - 0 [0 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 5 [100 %] ;

Class of Yb3S4 :
number of objects - 1 ;
correctly - 1 [100 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 0 [0 %] ;

Class of Yb3Se4 :
number of objects - 1 ;
correctly - 0 [0 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 1 [100 %] ;

Class of CaFe2O4 :
number of objects - 5 ;
correctly - 0 [0 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 5 [100 %] ;

```
Class of another structure :
        number of objects - 1 ;
        correctly         - 0 [ 0 % ] ;
        incorrectly       - 0 [ 0 % ] ;
        indeterminately   - 1 [ 100 % ] ;

Class without compound AB2Se4 :
        number of objects - 3 ;
        correctly         - 2 [ 66.666667 % ] ;
        incorrectly       - 0 [ 0 % ] ;
        indeterminately   - 1 [ 33.333333 % ] ;

Number of objects - 25 ;
correctly         - 4 [ 16 % ] ;
incorrectly       - 0 [ 0 % ] ;
indeterminately   - 21 [ 84 % ].
```

3.4.6. Predictions of Crystal Structure

The table of predictions of the crystal structure type for the compounds of composition $A(II)B(III)_2Se_4$ (Table 3.4.7) results from the comparison of the results of prediction with use of the descriptions in terms of the Features Sets I-III (see Section 2.6.3). The following designations are used:

S - spinel;
C - chalcopyrite;
P - $PbGa_2Se_4$;
Y - Yb_3S_4 ;
E - Yb_3Se_4 ;
F - $CaFe_2O_4$;
T - Th_3P_4 ;
O - olivine;

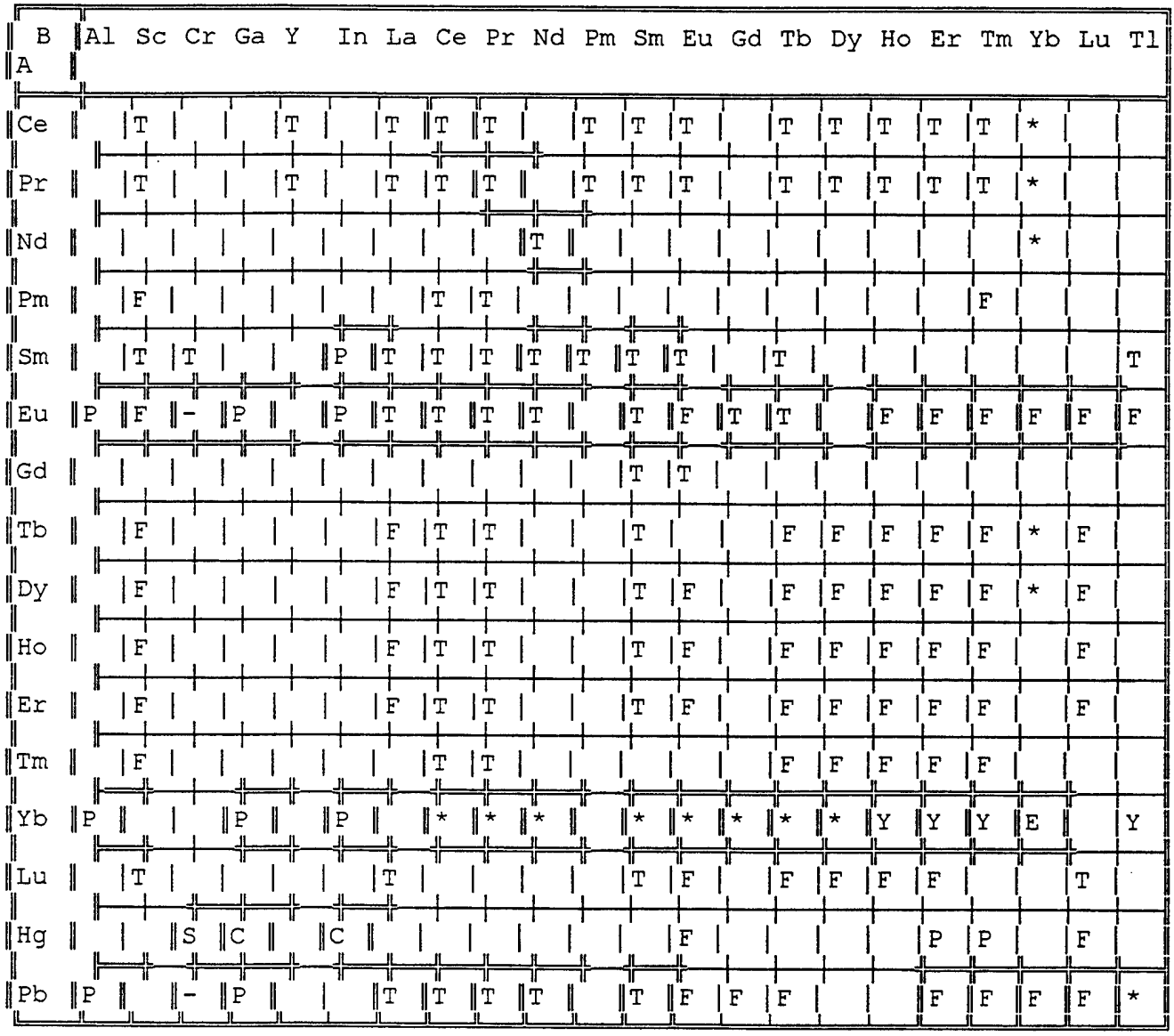
N - $NiCr_2Se_4$;
\- - the crystal structure differing from those listed above;
* - the compound of composition AB_2Se_4 does not form.

The physical-chemical systems, which were investigated experimentally, were outlined by double lines. The empty square corresponds to the lack of coincidence of the predictions, which have been obtained using different feature sets. According to our results the new compo-

unds of the composition $A(IV)B(II)_2Se_4$ with the crystal structure of the chalcopyrite, spinel, or Th_3P_4 at normal pressure and room temperature don't exist. The analysis of Table 3.4.7 shows: it is unlikely that the new compounds of the composition $A(II)B(III)_2Se_4$ with the crystal structure of the chalcopyrite or spinel form at normal pressure for the combinations of elements A and B which are indicated in this Table. At the same time the great number of predictions of new compounds with crystal structure type Th_3P_4, which hold the promise for searching for new electro-optical materials, were obtained.

Table 3.4.7
Table of Predictions of Crystal Structure Type
for Compounds of Composition $A(II)B(III)_2Se_4$

A \ B	Al	Sc	Cr	Ga	Y	In	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Tl
Mg	-					-	T															
Ca	P			P	Y	-	T									E	Y	E		E	E	
Ti		N	N																			
V		N	N																			
Cr		N	N			*	T	T	T	T		T	T		-	-					-	
Mn		S		-		-	T															
Fe		N		S																		
Co						*																
Ni			N																			
Cu			S	-		*				*				*						*		
Zn	C		S	C		C	T															
Sr	P			-	P	F		T								F	F	F	F	F	F	F
Y	T				T		T	T	T			T								*	T	
Cd	C		S	C	S	C	T		T					T		S	S	S	S	S	S	-
Ba	-			-	P	F		T					F		F		F				F	F	-
La		T	T						T	T			T			F	F	F	F				F



A \ B	Al	Sc	Cr	Ga	Y	In	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu	Tl
Ce	T			T		T	T	T		T	T	T		T	T	T	T	T	*			
Pr	T			T		T	T	T		T	T	T		T	T	T	T	T	*			
Nd									T										*			
Pm	F						T	T										F				
Sm	T	T				P	T	T	T	T	T	T	T		T							T
Eu	P	F	-	P		P	T	T	T	T		T	F	T	T		F	F	F	F	F	F
Gd												T	T									
Tb	F					F	T	T			T			F	F	F	F	F	*	F		
Dy	F					F	T	T			T	F		F	F	F	F	F	*	F		
Ho	F					F	T	T			T	F		F	F	F	F	F		F		
Er	F					F	T	T			T	F		F	F	F	F	F		F		
Tm	F						T	T						F	F	F	F	F				
Yb	P			P		P		*	*	*		*	*	*	*	*	Y	Y	Y	E		Y
Lu	T					T					T	F		F	F	F	F			T		
Hg		S	C		C							F					P	P		F		
Pb	P		-	P			T	T	T	T		T	F	F	F			F	F	F	F	*

3.5. Prediction of the New Compounds of Composition ABX_2.

The class of compounds with structure resembling that of chalcopyrite holds the greatest promise for searching for the new electro-optical and semiconducting materials [24,35]. We had attempted to predict the new chalcopyrites previously [37].

3.5.1. Prediction of New Chalcopyrites of Composition ABX_2

Prediction of New Chalcopyrites of Composition ABX_2 where:
(A = Li, Na, K, Rb, Cs, Cu, Ag, Au, Zn, Cd, Hg;
B = Al, Ga, In, Tl, Fe, Co, Ni; X = O, S, Se, Te)

3.5.1.1. Data for Computer Learning

The data for computer learning was extracted from the database on ternary inorganic compound properties [18-21]. In this investigation we attempted to predict new compounds with the composition given above which have the crystal structure resembling the chalcopyrite (space group I4(-)2d) [35], alfa-$NaFeO_2$(space group R3m) [29], beta-$NaFeO_2$ (space group $Pna2_1$), TlSe (space group I4/mcm) [38], or alfa-$LiFeO_2$ (space group $I4_1/amd$) at normal pressure and room temperature. Table 3.5.1 contains a learning set.

Table 3.5.1
Learning set for Prediction of Crystal Types of Compounds with Composition ABX_2

Composition	Crystal type
LiInTe2	chalcopyrite
CuAlS2	chalcopyrite
CuAlSe2	chalcopyrite
CuAlTe2	chalcopyrite
CuGaS2	chalcopyrite
CuGaSe2	chalcopyrite
CuGaTe2	chalcopyrite
CuInS2	chalcopyrite
CuInSe2	chalcopyrite
CuInTe2	chalcopyrite
CuTlS2	chalcopyrite
CuTlSe2	chalcopyrite
CuTlTe2	chalcopyrite
CuFeS2	chalcopyrite
CuFeSe2	chalcopyrite
CuFeTe2	chalcopyrite
AgAlS2	chalcopyrite
AgAlSe2	chalcopyrite
AgAlTe2	chalcopyrite
AgGaS2	chalcopyrite
AgGaSe2	chalcopyrite
AgGaTe2	chalcopyrite
AgInS2	chalcopyrite
AgInSe2	chalcopyrite
AgInTe2	chalcopyrite
AgTlSe2	chalcopyrite
AgTlTe2	chalcopyrite
AgFeO2	chalcopyrite
AgFeS2	chalcopyrite
AgFeSe2	chalcopyrite
AgFeTe2	chalcopyrite
ZnAlS2	chalcopyrite

Composition	Crystal type
ZnAlSe2	chalcopyrite
ZnAlTe2	chalcopyrite
ZnGaTe2	chalcopyrite
ZnTlTe2	chalcopyrite
CdGaTe2	chalcopyrite
HgGaTe2	chalcopyrite
LiAlS2	beta-NaFeO2
LiGaO2	beta-NaFeO2
LiInSe2	beta-NaFeO2
NaAlO2	beta-NaFeO2
NaGaO2	beta-NaFeO2
LiAlO2	alfa-NaFeO2
LiNiO2	alfa-NaFeO2
NaInS2	alfa-NaFeO2
NaInSe2	alfa-NaFeO2
NaInO2	alfa-NaFeO2
NaTlO2	alfa-NaFeO2
NaFeO2	alfa-NaFeO2
NaCoO2	alfa-NaFeO2
NaNiO2	alfa-NaFeO2
KInO2	alfa-NaFeO2
KTlO2	alfa-NaFeO2
RbInO2	alfa-NaFeO2
RbTlO2	alfa-NaFeO2
CsTlO2	alfa-NaFeO2
CuAlO2	alfa-NaFeO2
CuGaO2	alfa-NaFeO2
CuFeO2	alfa-NaFeO2
CuCoO2	alfa-NaFeO2
AgGaO2	alfa-NaFeO2
AgInO2	alfa-NaFeO2
AgTlO2	alfa-NaFeO2
AgCoO2	alfa-NaFeO2
AgNiO2	alfa-NaFeO2
AgNiSe2	alfa-NaFeO2
AgNiTe2	alfa-NaFeO2
NaAlSe2	TlSe
NaAlTe2	TlSe
NaGaTe2	TlSe
NaInTe2	TlSe
KAlTe2	TlSe
KInTe2	TlSe
CdTlSe2	TlSe
LiInO2	alfa-LiFeO2
LiTlO2	alfa-LiFeO2
LiFeO2	alfa-LiFeO2

Composition	Crystal type	Space group	Z
NaNiSe2	NaCl	Fm3m	
KAlSe2	KAlSe2	P1	32
KAlO2		Pbca	
KGaS2		Aa	16
KGaSe2		P1	32
KGaTe2		P1	32
KGaO2		Pbca	16
KInS2	RbInS2	Cc	16
KInSe2		P1	32
KTlS2	RbInS2	Cc	16
KFeO2	KFeO2	P2(1)nb	16
KFeS2		C2/c	4
KFeSe2		C2/c	4
KCoO2		tetragonal	2
RbGaO2	KFeO2	P2(1)nb	16
RbInS2	RbInS2	Cc	16
RbTlS2	RbInS2	Cc	16
RbFeS2		C2/c	4
RbFeSe2		C2/c	4
RbCoO2		Pbca	16
CsAlO2		Fd3m	
CsGaS2		C2/c	4
CsInS2	RbInS2	Cc	16
CsTlS2	RbInS2	Cc	16
CsFeS2		Immm	4
CsFeSe2		monoclinic	
CuNiS2		cubic	
AgAlO2		P6(3)/mmc	
CdInS2	CdTlS2	P3(-)m1	1
CdTlS2	CdTlS2	P3(-)m1	1
HgTlS2		I4/mmm	8

Pseudo-Binary Systems in which Compound of Composition ABX_2 does not Form

ZnS-TlS	without	compound ABX2
ZnO-FeO	without	compound ABX2
ZnO-CoO	without	compound ABX2
ZnO-NiO	without	compound ABX2
HgSe-TlSe	without	compound ABX2

3.5.1.2. Selection of Features

On the basis of physical-chemical grounds two sets of chemical element features were selected for the description of oxide and chalcogenide compounds.

3.5.1.2.1. First Feature Set

The first feature set coincides with Set I (see Section 3.4.2.1).

3.5.1.2.2. Set of Properties for Feature Set IV

The set of properties of chemical elements for Feature Set IV includes the following information: the types of incomplete electronic shells of separate atoms, the isobaric thermal capacities at 298 K, the ionic radii, the first four ionization potentials, the electronegatives by Pauling, the energies of the crystal lattice, the temperatures and the heats of melting, the entropies of the individual substances at 298 K, Debye (characteristic) temperatures, and the formal valence of the elements A, B, or X represented in the compound of composition ABX_2. The quantitative properties were quantized on the basis of the uniform distribution of the interval values. Table 3.5.2 contains the gradations for Feature Set IV.

Table 3.5.2
Gradations for the Feature Set IV

Feature	Gradation	Feature	Gradation
Type of incomplete electronic shell		Energy of the crystal lattice,	
s	S	-6	
p	P	E*10 J/kg*mol	
d	D	[79-130]	E1
f	F	(130-182.8]	E2
Electronegative		(182.8-244]	E3
		(244-315.5]	E4
[0.7-0.8]	X1	(315.5-356.1]	E5
(0.8-1.09]	X2	(356.1-364.7]	E6
(1.09-1.2]	X3	(364.7-408]	E7
(1.2-1.3]	X4	(408-524]	E8
(1.3-1.5]	X5	(524-652]	E9
(1.5-1.7]	X6	(652-905]	E10
(1.7-1.8]	X7	Debye	

Feature	Gradation	Feature	Gradation
(1.8-2]	X8	temperature, K	
(2-2.2]	X9	[39.2-90]	TD1
(2.2-2.9]	X10	(90-129]	TD2
(2.9-4]	X11	(129-153]	TD3
First		(153-163]	TD4
ionization		(163-190]	TD5
potential		(190-233]	TD6
[3.893-5.39]	I11	(233-310]	TD7
(5.39-5.90]	I12	(310-405]	TD8
(5.90-6.31]	I13	(405-465]	TD9
(6.31-6.74]	I14	(465-585]	TD10
(6.74-6.95]	I15	(585-1860]	TD11
(6.95-7.432]	I16	Melting	
(7.432-7.87]	I17	point, K	
(7.87-8.64]	I18	[13.9-303]	TM1
(8.64-9.30]	I19	(303-527]	TM2
(9.30-10.55]	I110	(527-870]	TM3
(10.55-25]	I111	(870-1090]	TM4
Second		(1090-1323]	TM5
ionization		(1323-1629]	TM6
potential, eV		(1629-1823]	TM7
[0-11.5]	I21	(1823-2473]	TM8
(11.5-12.4]	I22	(2473-3660]	TM9
(12.4-14.2]	I23	Heat of	
(14.2-15.92]	I24	melting,	
(15.92-16.904]	I25	kJ/mol	
(16.904-18.7]	I26	[0.1-2.2]	H1
(18.7-19.65]	I27	(2.2-4.6]	H2
(19.65-21.5]	I28	(4.6-8.3]	H3
(21.5-27.56]	I29	(8.3-10.9]	H4
(27.56-75.62]	I210	(10.9-13.8]	H5
Third		(13.8-15.7]	H6
ionization		(15.7-17.6]	H7
potential, eV		(17.6-23.9]	H8
[0-21]	I31	(23.9-27.7]	H9
(21-24]	I32	(27.7-35.4]	H10
(24-25.61]	I33	Formal	
(25.61-29]	I34	valency	
(29-30.64]	I35	0	B0
(30.64-32.8]	I36	+1	B1
(32.8-34.21]	I37	+2	B2
(34.21-37]	I38	+3	B3
(37-47.426]	I39	+4	B4
(47.426-154]	I310	+5	B5
Fourth		+6	B6
ionization		+7	B7
potential, eV		+8	B8
[0-36.7]	I41	-1	B1-

Feature	Gradation	Feature	Gradation
(36.7-41]	I42	-2	B2-
(41-44]	I43	-3	B3-
(44-46]	I44	-4	B4-
(46-48]	I45	-5	B5-
(48-52]	I46	-6	B6-
(52-56]	I47	-7	B7-
(56-64.2]	I48	Entropies of	
(64.2-97.16]	I49	individual	
(97.16-259.3]	I410	substances	
Ionic		at 298 K,	
radius, A		kJ/kg*mol*K	
[0-0.39]	R1	[5.73-27.1]	S1
(0.39-0.57]	R2	(27.1-30.7]	S2
(0.37-0.65]	R3	(30.7-32.8]	S3
(0.65-0.69]	R4	(32.8-38]	S4
(0.69-0.78]	R5	(38-43]	S5
(0.78-0.85]	R6	(43-51]	S6
(0.85-0.90]	R7	(51-58]	S7
(0.90-0.99]	R8	(58-69]	S8
(0.99-1.11]	R9	(69-74]	S9
(1.11-2.20]	R10	(74-95]	S10
Isobaric		(95-152]	S11
thermal		(152-224]	S12
capacity			
at 298 K,			
kj/kg*mol*K			
[7-20.808]	C1		
(20.808-23.41]	C2		
(23.41-24.79]	C3		
(24.79-25.246]	C4		
(25.246-26]	C5		
(26-26.377]	C6		
(26.377-27.18]	C7		
(27.18-28.01]	C8		
(28.01-31.359]	C9		
(31.359-95]	C10		

3.5.1.3. Computer Learning

Computer learning is carried out for two learning sets in which the compounds from Table 3.5.1 were described in terms of the sets of the component properties I and IV. The system of concept formation CONFOR [14] was used for the computer learning and prediction. The pyramidal networks and the corresponding logical expressions were formed as a result of computer learning via CONFOR. Appendix 2 contains the logical expressions for various learning sets.

3.5.1.4. Analyse of Semantic Network and Corresponding Logical Expression

The aim of analyse is a search for the most important combinations (conjunctions) of component property bins which determine the classes to a considerable extent. Special procedure of CONFOR is intended for solution of this problem. It allows to find the component property values which are the most characteristic of certain class. Table 3.5.3 contains the results of such an analyse for various classes.

Table 3.5.3
Result of Analyse of Pyramidal Network (Feature Set IV)

Conjunction	Number of recurrences
Chalkopyrite	
S, R10, P, B2-	38
S, R10, P, B2-, B1, B3	31
S, R10, P, B2-, B1, E3	30
I17, I38	30
I17, I38, I28	30
I17, I38, I28, H5	30
beta-$NaFeO_2$	
S, R10, P, B2-	5
S, R10, P, B2-, B1, B3	5
I210, I310	5
I210, I310, I11	5
S, R10, P, B2-, B1, B3, I210, I310	5
alpha-$NaFeO_2$	
S, R10, P, B2-	25
S, R10, P, B2-, B1, B3	25
I210, I310	23
S, R10, P, B2-, B1, B3, I210, I310	23
S, R10, P, B2-, B1, B3, I210, I310, I49	23
TM1, C9	21
TM1, C9, I111, S12, B6	21
TM1, C9, I111, S12, B6, H1	21
S, R10, P, B2-, B1, B3, I210, I310, I49, TM1, C9, I111, S12, B6, H1	21

Conjunction	Number of recurrences
TlSe	
C5, I36	7
S, R10, P, B2-	7
E1, H2	7
S, R10, P, B2-, TM3	7
S, R10, P, B2-, B1, B3	6
S, R10, P, B2-, B1, B3, E3	6
E3, I27	6
I11, C9	6
I11, C9, I210	6
R8, S7	6
E1, H2, R8, S7	6
Without compound ABX_2	
C5, H3	5
S, R10, P, B2-	5
S, R10, P, B2-, TM3	5
S, R10, P, B2-, TM3, I110	5

Analyse of Table 3.5.3 shows that the chalkopyrites contain at least one element having first ionization potential in the range from 7.432 to 7.87 eV, second ionization potential in the range from 19.65 to 21.5 eV, and third ionization potential in the range from 34.21 to 37 eV, and its heat of melting must be in the range between 10.9 and 13.8 kJ/mol. The fields of crystal structure types alpha- and beta-$NaFeO_2$ intersect. But compounds with structure type TlSe contain at least one element having third ionization potential in the range from 30.64 to 32.8 eV and standard capacity in the range from 25.246 to 26 kJ/kg*mol*K, or energy of the crystal lattice in the range between $79*10^{-6}$ - $130*10^{-6}$ J/kg*mol and heat of melting in the range from 2.2 to 4.6 kJ/mol, and so forth. A distinguishing characteristic of class "without compound ABX2" is a presence in physico-chemical system at least one element with standard capacity in the range from 25.246 to 26 kJ/kg*mol*K and the heat of melting in the range from 4.6 to 8.3 kJ/mol. Conjunctions S & R10 & P & B2- , S & R10 & P & B2- & B1 & B3 characterize all classes and don't be dividing.

3.5.1.5. Prediction of Crystal Structure

The table of predictions of crystal structure type for the compounds with composition ABX_2 (Table 3.5.4) comes from the comparison of the results of prediction with use of the descriptions in terms of the Feature Sets I and IV (see Section 1.6.3). The following designations are used:

C - chalcopyrite;
N - alfa-$NaFeO_2$;
B - beta-$NaFeO_2$;
L - alfa-$LiFeO_2$;
T - TlSe;
- - the crystal structure differing from those listed above;
* - the compound of composition ABX_2 does not form.

Physical-chemical systems, have been investigated experimentally and used for computer learning, were outlined by double lines. The empty square corresponds to the lack of coincidence of the predictions, which have been obtained using different feature sets. The analysis of Table 3.5.4 shows that few new compounds of the composition ABX_2 with the crystal structure of chalcopyrite form at normal pressure. The most reliable predictions of the chalcopyrite structure were obtained for compounds of composition $HgFeSe_2$, $HgCoSe_2$, and $HgNiSe_2$. These predictions were obtained using two feature sets. At the same time the predictions of the structure type of chalcopyrite for compounds with composition $ZnGaSe_2$, $RbInTe_2$, $KTlTe_2$, $RbTlTe_2$, $CdTlTe_2$, $HgFeO_2$, $KFeTe_2$, $RbFeTe_2$, $HgCoO_2$, $CoCoS_2$, $KCoTe_2$, $RbCoTe_2$, and $HgNiO_2$ were obtained only for one feature set (the use of another set had given an unrecognized result). The analysis of Table 3.5.4 shows also that the volume of the learning set is too small for reliable prediction of new chalcopyrites of composition ABX_2.

Table 3.5.4
Crystal Types of Compounds with Composition ABX_2

A \ X	B=Al O	B=Al S	B=Al Se	B=Al Te	B=Ga O	B=Ga S	B=Ga Se	B=Ga Te	B=In O	B=In S	B=In Se	B=In Te	B=Tl O	B=Tl S	B=Tl Se	B=Tl Te	B=Fe O	B=Fe S	B=Fe Se	B=Fe Te	B=Co O	B=Co S	B=Co Se	B=Co Te	B=Ni O	B=Ni S	B=Ni Se	B=Ni Te
Li	N	B			B				L		B	C	L				L								N			
Na	B		T	T	B			T	N	N	N	T	N				N				N				N	T	-	T
K	-		-	T	-	-	-	-	N	-	-	T	N	-		C	-	-	-	C	-	-		C				
Rb	-				-				N	-		C	N	-		C	-	-	-	C	-	-	-	C	-	T	-	
Cs	-					-				-			N	-			-	-	-		-	-	-		-		-	T
Cu	N	C	C	C	N	C	C	C		C	C	C		C	C	C	N	C	C	C	N	C			N	-		
Ag	-	C	C	C	N	C	C	C	N	C	C	C	N		C	C	C	C	C	C	N				N	N	N	N
Au										-							L	-			L	-	-		L	T	-	T
Zn	-	C	C	C	-	-	C	C	-	-	-	-		*		C	*	-			*	-			*	-		
Cd	-	-				-	-	C	T	-	-			-	T	C	T	-			T	-			T	-		
Hg				-		-		C	C			-		-	*		C		C		C		C		C		C	

3.5.2. Prediction of New Chalcopyrites w/Composition ABX_2 and CDY_2

Prediction of New Chalcopyrites of the Composition ABX_2 and CDY_2 :

A = Mg, Ca, Sr, Ba, Zn, Cd, Hg; B = Si, Ge, Sn; X = N, P, As, Sb, Bi, S, Se, Te; C = Li, Na, K, Rb, Cs; D = P, As, Sb, Bi; Y = N, P, As, Sb, Bi.

3.5.2.1. Data for Computer Learning

The data for computer learning was extracted from the DB on ternary inorganic compound properties [18-21]. In this investigation we attempted to predict new compounds with composition given above which have the crystal structure resembling that of chalcopyrite (space group I4(-)2d) [35] and beta-$NaFeO_2$ (space group $Pna2_1$) at normal pressure and room temperature. Table 3.5.5 contains a learning set.

Table 3.5.5
Learning Set for Predicting Crystal Types of Compounds with Composition ABX_2

Composition	Crystal type
MgSiP2	chalcopyrite
ZnSiP2	chalcopyrite
CdSiP2	chalcopyrite
ZnSiAs2	chalcopyrite
CdSiAs2	chalcopyrite
ZnGeP2	chalcopyrite
ZnGeAs2	chalcopyrite
CdGeP2	chalcopyrite
CdGeAs2	chalcopyrite
CdGeTe2	chalcopyrite
ZnSnP2	chalcopyrite
ZnSnAs2	chalcopyrite
ZnSnSb2	chalcopyrite
CdSnP2	chalcopyrite
CdSnAs2	chalcopyrite
CaGeN2	chalcopyrite
LiPN2	chalcopyrite
MgSiN2	beta-NaFeO2
MgGeN2	beta-NaFeO2
ZnGeN2	beta-NaFeO2

Composition	Crystal type	Space group	Z
MgGeP2	ZnS		
BaSnS2		P2(1)/c	4
NaPN2		I4(-)	4

Ternary Systems in which Compound of Composition ABX_2 does not Form

Cd-Sn-Sb	without	compound	AB2Se4
Cd-Sn-Bi	without	compound	AB2Se4
Cd-Sn-S	without	compound	AB2Se4
Cd-Sn-Se	without	compound	AB2Se4
Cd-Sn-Te	without	compound	AB2Se4
Hg-Sn-Bi	without	compound	AB2Se4
Hg-Sn-S	without	compound	AB2Se4
Hg-Sn-Se	without	compound	AB2Se4
Hg-Sn-Te	without	compound	AB2Se4
Mg-Si-Sb	without	compound	AB2Se4
Cd-Si-Te	without	compound	AB2Se4
Zn-Ge-Te	without	compound	AB2Se4
Cd-Ge-Se	without	compound	AB2Se4
Hg-Ge-S	without	compound	AB2Se4
Hg-Ge-Se	without	compound	AB2Se4
Hg-Ge-Te	without	compound	AB2Se4
Mg-Sn-Sb	without	compound	AB2Se4
Mg-Sn-Bi	without	compound	AB2Se4
Ca-Sn-S	without	compound	AB2Se4
Zn-Sn-Se	without	compound	AB2Se4
Zn-Sn-Te	without	compound	AB2Se4

On the basis of physical-chemical grounds two sets of chemical element features were selected. The first feature set coincides with Set I (see Section 3.4.2.1) but does not include the formal valence of elements, because it is difficult to determine one for the compounds of this kind. The second feature set coincides with Set IV (see Section 3.5.1.2.2), but instead of ionic radii, the covalent radii were included. See in Table 3.5.6 the gradations for the covalent radii. In addition, the formal valence of elements was excluded also.

Table 3.5.6
The gradations for covalent radii, A

Feature	Gradation
[0.28-0.66]	RC1
(0.66-0.77]	RC2
(0.77-1.00]	RC3
(1.00-1.14]	RC4
(1.14-1.22]	RC5
(1.22-1.27]	RC6
(1.27-1.33]	RC7
(1.33-1.40]	RC8
(1.40-1.54]	RC9

3.5.2.2. Computer Learning

The computer learning is carried out for two learning sets in which the compounds from Table 3.5.5 were described in terms of the feature sets of the component properties I and IV with alterations. The system of concept formation CONFOR [14] was used for the computer learning and predicting. Two pyramidal networks and the corresponding logical expressions were formed as a result of computer learning. Appendix 3 contains the logical expressions for various learning sets.

3.5.2.3. Analyse of Semantic Network and Corresponding Logical Expression

Table 3.5.7 contains the results of analyse for various classes.

Table 3.5.7
Result of Analyse of Pyramidal Network (Feature Set IV with Covalent Radii)

Conjunction	Number of recurrences
Chalkopyrite	
S, P	17
S, P, TM3	16
C1, H3	15
S, P, TM3, C1, H3	15
I110, E4	15
beta-$NaFeO_2$	
TD8, S3	3
S, P	3
TD8, E2	3
S, P, H1	3
C9, TM1	3
S, P, H1, C9, TM1	3
S, P, H1, C9, TM1, RC2, I111, I210, I39, I49, S12	3
I25, I44	3
I25, I44, I18	3
I25, I44, I18, I37	3
I25, I44, I18, I37, RC5	3
TD8, E2, I25, I44, I18, I37, RC5	3
Without compound ABX_2	
S, P	21
RC8, I36	17
RC8, I36, C2	16
TD5, S7	16
RC88, I24	15
TM2, I45	15
TD5, TM2, I45	15

Analyse of Table 3.5.7 shows that the chalkopyrites contain at least one element having standard entropy in the range from 30.7 to 32.8 kJ/kg*mol*K and heat of melting must be in the range between 4.6 and 8.3 kJ/mol, or first ionization potential in the range from 9.30 to 10.55 eV and energy of the crystal lattice in the range between $244*10^{-6}$ and $315.5*10^{-6}$ J/kg*mol. The compounds with structure type of beta-$NaFeO_2$ contain at least one element having Debye temperature in the range from 310 to 405 K and standard capacity in the range from 23.41 to 24.79 kJ/kg*mol*K, or Debye temperature in the range from 310 to 405 K and energy of the crystal lattice in the range between $130*10^{-6}$ and $182.8*10^{-6}$ J/kg*mol, and so forth. A distinguishing characteristic of class "without compound ABX2" is a presence in physico-chemical system at least one element with covalent radius in the range from 1.33 to 1.40 A and the third ionization potential in the range from 30.64 to 32.8 eV, and standard capacity in the range from 20.808 to 23.41 kJ/kg*mol*K, or Debye temperature in the range from 163 to 190 K and standard entropy in the range from 51 to 58 kJ/kg*mol*K, and so forth. Conjunction S & P characterizes all classes and don't be dividing.

3.5.2.4. Predictions of Crystal Structure

The tables of predictions of the crystal structure type for the compounds of the composition ABX_2 (Tables 3.5.8 and 3.5.9) result from the comparison of the results of prediction with descriptions in terms of the feature sets I and IV (with alterations). See designations in Section 3.5.1.5.

Table 3.5.8
Crystal Types of Compounds with Composition ABX_2

	B=Si								B=Ge								B=Sn							
X / A	N	P	As	Sb	Bi	S	Se	Te	N	P	As	Sb	Bi	S	Se	Te	N	P	As	Sb	Bi	S	Se	Te
Mg	B	C	*	*	*	*	*	*	B	-	C	C	*	*	*	*			*	*	*	-	*	
Ca	B	-	*	*		*	*	*	C	-	C	C	*	*	*	*					C	*		
Sr			*	*		*	*	*	B	-	C	C	*	*	*	*			*	*		-	*	
Ba			*	*		*	*	*	B	-	C	C	*	*	*	*			*	*	*	-	*	*
Zn		C	C	*				*	B	C	C	B				*	C	C	C	C			*	*
Cd		C	C	*	*	*	*	*		C	C	*	*	*	*	C		C	C	*	*	*	*	*
Hg			*	*		*	*	*	B	-	C	C	*	*	*	*		*	*	*	*	*	*	*

Table 3.5.9
Crystal Types of Compounds with Composition ABX_2

	B=P					B=As					B=Sb					B=Bi				
A \ X	N	P	As	Sb	Bi	N	P	As	Sb	Bi	N	P	As	Sb	Bi	N	P	As	Sb	Bi
Li	C	-				B			C		B		C							
Na	-	-	-	-		B	-		C	*	B	-	C		*			*	*	
K	C	-	-	-		B	-		C	*	B	-	C		*			*	*	
Rb		-	-	-		B	-		B		B	-	B							
Cs		-	-	-		B	-		B		B	-	B		*				*	

The analysis of Tables 3.5.8 and 3.5.9 shows that few new compounds of the composition ABX_2 with the crystal structure of the chalcopyrite form at normal pressure. We did not obtain the predictions of chalcopyrite structure using the two feature sets. The predictions of the chalcopyrite structure type for compounds with composition $MgGeAs_2$, $MgGeSb_2$, $CaGeAs_2$, $CaGeSb_2$, $CaSnBi_2$, $SrGeAs_2$, $SrGeSb_2$, $BaGeAs_2$, $BaGeSb_2$, $HgGeAs_2$, $HgGeSb_2$, KPN_2, $LiAsSb_2$, $NaAsSb_2$, $LiSbAs_2$, $NaSbAs_2$, $KSbAs_2$, and $KAsSb_2$, were obtained only for one feature set (the use of another set had given an unrecognized result). These predictions are not reliable. The analysis of these Tables shows also that the volume of the learning set is too small for reliable prediction of new chalcopyrites with composition ABX_2.

3.6. Prediction of New Compounds of Composition $A^{I}{}_3B^{II}Cl_5$

The class of compounds with composition A_3BCl_5 holds the promise for searching for the new IR-elecro-acousto-optical materials [24].

3.6.1. Data for Computer Learning

The data for computer learning was extracted from the DB on ternary inorganic compound properties [18-21]. In this investigation we succeeded to predict only the possibility of formation of new compounds with this composition, because the number of examples for prediction of crystal structure types was too small for computer learning of high quality. The table 3.6.1 contains a learning set.

Table 3.6.1
Learning Set for Prediction of the Possibility of Forming Compounds with Composition A_3BCl_5

Composition	Crystal type	Space group
Na3CrCl5		
Rb3MgCl5		
Cs3MgCl5		
K3TiCl5		
K3BaCl5		
Cs3MnCl5	Cs3CoCl5	I4/mcm, Z=4
Rb3FeCl5	Cs3CoCl5	I4/mcm, Z=4
Cs3FeCl5	Cs3CoCl5	I4/mcm, Z=4
Cs3CoCl5	Cs3CoCl5	I4/mcm, Z=4
Tl3CoCl5	Cs3CoCl5	I4/mcm, Z=4
Cs3NiCl5	Cs3CoCl5	I4/mcm, Z=4
Cs3ZnCl5	Cs3CoCl5	I4/mcm, Z=4
Tl3ZnCl5		
Rb3SrCl5		
Rb3CdCl5		
Tl3PdCl5		Pbca, Z=8
Cs3CdCl5	Cs3CoCl5	I4/mcm, Z=4
Tl3CdCl5		
Tl3SnCl5		
Cs3BaCl5		
Cs3HgCl5		
Tl3PbCl5		alfa: P4(1), Z=4; beta: P2(1)2(1)2(1)

Pseudo-Binary Systems in which Compound of Composition A_3BCl_5 does not Form

LiCl-MgCl2	without compound A3BCl5
LiCl-CaCl2	without compound A3BCl5
LiCl-VCl2	without compound A3BCl5
LiCl-MnCl2	without compound A3BCl5
LiCl-FeCl2	without compound A3BCl5
LiCl-NiCl2	without compound A3BCl5
LiCl-CuCl2	without compound A3BCl5
LiCl-ZnCl2	without compound A3BCl5
LiCl-SrCl2	without compound A3BCl5
LiCl-PdCl2	without compound A3BCl5
LiCl-CdCl2	without compound A3BCl5
LiCl-SnCl2	without compound A3BCl5
LiCl-BaCl2	without compound A3BCl5
LiCl-SmCl2	without compound A3BCl5
LiCl-EuCl2	without compound A3BCl5
LiCl-PbCl2	without compound A3BCl5

Composition	Crystal type	Space group
NaCl-BeCl2	without compound A3BC15	
AgCl-BeCl2	without compound A3BC15	
RbCl-BeCl2	without compound A3BC15	
CsCl-BeCl2	without compound A3BC15	
NaCl-MgCl2	without compound A3BC15	
NaCl-CaCl2	without compound A3BC15	
NaCl-TiCl2	without compound A3BC15	
NaCl-MnCl2	without compound A3BC15	
NaCl-FeCl2	without compound A3BC15	
NaCl-CoCl2	without compound A3BC15	
NaCl-NiCl2	without compound A3BC15	
NaCl-CuCl2	without compound A3BC15	
NaCl-ZnCl2	without compound A3BC15	
NaCl-SrCl2	without compound A3BC15	
NaCl-PdCl2	without compound A3BC15	
NaCl-CdCl2	without compound A3BC15	
NaCl-SnCl2	without compound A3BC15	
NaCl-BaCl2	without compound A3BC15	
NaCl-SmCl2	without compound A3BC15	
NaCl-EuCl2	without compound A3BC15	
NaCl-YbCl2	without compound A3BC15	
NaCl-PbCl2	without compound A3BC15	
KCl-MgCl2	without compound A3BC15	
CuCl-MgCl2	without compound A3BC15	
AgCl-MgCl2	without compound A3BC15	
TlCl-MgCl2	without compound A3BC15	
KCl-CaCl2	without compound A3BC15	
KCl-VCl2	without compound A3BC15	
KCl-CrCl2	without compound A3BC15	
KCl-MnCl2	without compound A3BC15	
KCl-FeCl2	without compound A3BC15	
KCl-CoCl2	without compound A3BC15	
KCl-NiCl2	without compound A3BC15	
KCl-SrCl2	without compound A3BC15	
KCl-PdCl2	without compound A3BC15	
KCl-CdCl2	without compound A3BC15	
KCl-SnCl2	without compound A3BC15	
KCl-SmCl2	without compound A3BC15	
KCl-EuCl2	without compound A3BC15	
KCl-YbCl2	without compound A3BC15	
KCl-PbCl2	without compound A3BC15	
CuCl-CaCl2	without compound A3BC15	
RbCl-CaCl2	without compound A3BC15	
AgCl-CaCl2	without compound A3BC15	
CsCl-CaCl2	without compound A3BC15	
CsCl-TiCl2	without compound A3BC15	
CsCl-VCl2	without compound A3BC15	
RbCl-CrCl2	without compound A3BC15	

Composition	Crystal type	Space group
CsCl-CrCl2	without compound A3BC15	
RbCl-MnCl2	without compound A3BC15	
AgCl-MnCl2	without compound A3BC15	
TlCl-MnCl2	without compound A3BC15	
AgCl-CoCl2	without compound A3BC15	
AgCl-NiCl2	without compound A3BC15	
CuCl-ZnCl2	without compound A3BC15	
CuCl-PdCl2	without compound A3BC15	
CuCl-SnCl2	without compound A3BC15	
CuCl-HgCl2	without compound A3BC15	
CuCl-PbCl2	without compound A3BC15	
RbCl-ZnCl2	without compound A3BC15	
AgCl-ZnCl2	without compound A3BC15	
RbCl-PdCl2	without compound A3BC15	
RbCl-SnCl2	without compound A3BC15	
RbCl-EuCl2	without compound A3BC15	
RbCl-PbCl2	without compound A3BC15	
AgCl-SrCl2	without compound A3BC15	
CsCl-SrCl2	without compound A3BC15	
TlCl-SrCl2	without compound A3BC15	
AgCl-PdCl2	without compound A3BC15	
CsCl-PdCl2	without compound A3BC15	
AgCl-CdCl2	without compound A3BC15	
AgCl-SnCl2	without compound A3BC15	
AgCl-BaCl2	without compound A3BC15	
AgCl-HgCl2	without compound A3BC15	
AgCl-PbCl2	without compound A3BC15	
CsCl-SnCl2	without compound A3BC15	
CsCl-EuCl2	without compound A3BC15	
TlCl-BaCl2	without compound A3BC15	
TlCl-EuCl2	without compound A3BC15	

3.6.2. Selection of Features

On the basis of physical-chemical grounds two sets of chemical elements features and set of simple chlorides feature were selected for the description of these systems.

The first feature set (feature set V) coincides with Set I (see Section 3.4.2.1), but instead of covalent radii of elements A and B, ionic radii were used for the description of the objects. The used gradations for the ionic radii are indicated in the table 3.5.2 (Gradations for Feature Set IV).

The second feature set coincides with the set IV (see Section 3.5.1. 2.2).

The third set of properties of simple chlorides (feature set VI) includes the following information: the temperatures melting for simple chlorides, the standard entropies at 298 K and the standard enthalpy of formation for corresponding simple chlorides, the ionic radii of the corresponding cations of elements A and B (Table 3.6.2). The properties were quantized on the basis of the uniform distribution of the values of the intervals. Table 3.6.2 contains the gradations for Feature Set VI.

Table 3.6.2
Gradations for Feature Set VI
(Properties of Simple Chlorides)

Feature	Gradation	Feature	Gradation
Melting point of chlorides, K		Standard enthalpy of formation for corresponding simple chlorides, kcal/mol	
[166-276]	TM1	[3-28.3]	H1
(276-450]	TM2	(28.3-45.6]	H2
(450-500]	TM3	(45.6-55]	H3
(500-561]	TM4	(55-77.4]	H4
(561-600]	TM5	(77.4-86.8]	H5
(600-728]	TM6	(86.8-98.3]	H6
(728-860]	TM7	(98.3-110]	H7
(860-923]	TM8	(110-126.4]	H8
(923-994]	TM9	(126.4-164.1]	H9
(994-1050]	TM10	(164.1-195.6]	H10
(1050-1100]	TM11	(195.6-228]	H11
(1100-1200]	TM12	(228-237.2]	H12
(1200-1623]	TM13	(237.2-245.8]	H13
Standard entropy for corresponding simple chlorides, cal/mol*K		(245.8-284.5]	H14
		Ionic radii, A	
[13.9-21]	S1	[0-0.61]	R1
(21-25.9]	S2	(0.61-0.65]	R2
(25.9-27.7]	S3	(0.65-0.69]	R3
(27.7-29.61]	S4	(0.69-0.78]	R4
(29.61-31.3]	S5	(0.78-0.82]	R5
(31.3-33.5]	S6	(0.82-0.86]	R6
(33.5-36.64]	S7	(0.86-0.90]	R7
(36.64-38.01]	S8	(0.90-0.97]	R8
(38.01-40.8]	S9	(0.97-1.02]	R9
(40.8-45.8]	S10	(1.02-1.20]	R10
(45.8-49]	S11	(1.20-1.65]	R11
(49-54]	S12		
(54-61.5]	S13		
(61.5-70.5]	S14		

3.6.3. Computer Learning

The computer learning is carried out for three learning sets in which the compounds from Table 3.6.1 were described in terms of the sets of the component properties V, IV and VI. The system of concept formation CONFOR [14] was used for computer learning and prediction.

The pyramidal networks and the corresponding logical expressions were formed as a result of computer learning via CONFOR. Appendix 4 contains the logical expressions for various learning sets.

3.6.4. Prediction of Formation

The table of predictions of possibility of forming compounds with composition $A^{I}{}_3B^{II}Cl_5$ (Table 3.6.3) results from comparison of the results of prediction with use of the descriptions in terms of the Features Sets IV, V and VI (see Section 1.6.3). The following designations are used:

+ - the compound of composition A_3BCl_5 forms;

- - the compound of composition A_3BCl_5 does not form.

The physical-chemical systems, which were investigated experimentally and used for computer learning, were outlined by double lines. The empty square corresponds to the lack of coincidence of the predictions, which have been obtained using different feature sets.

The analysis of Table 3.6.3 shows that few new compounds of the composition A_3BCl_5 form at normal pressure: In_3FeCl_5, Rb_3CoCl_5, and Tl_3CuCl_5.

Table 3.6.3
Table of Predictions
of Possibility of Forming
Compounds with Composition $A^{I}{}_3B^{II}Cl_5$

A / B	Li	Na	K	Cu	Rb	Ag	In	Cs	Tl
Be	-	-	-	-	-	-		-	-
Mg	-	-	-	-	+	-	-	+	-
Ca	-	-	-	-	-	-	-	-	
Ti		-	+	-	-	-	-	-	-
V	-		-	-	-	-		-	-
Cr	-	+	-		-	-	-	-	-

A / B	Li	Na	K	Cu	Rb	Ag	In	Cs	Tl
Mn	-	-	-	-	-	-		+	-
Fe	-	-	-	-	+	-	+	+	
Co		-	-	-	+	-	-	+	+
Ni	-	-	-	-		-	-	+	-
Cu	-	-	-	-	-	-	-		+
Zn	-	-		-	-	-		+	+
Ge	-	-		-	-	-		-	
Sr	-	-	-	-	+	-		-	-
Tc	-	-	-	-		-			
Pd	-	-	-	-	-	-		-	+
Cd	-	-	-	-	+	-		+	+
Sn	-	-	-	-	-	-		-	+
Ba	-	-	+	+		-		+	-
La	-	-	-	-		-			-
Sm	-	-	-	-	-	-			
Eu	-	-	-	-	-	-		-	-
Yb	-	-	-	-	-	-			-
Hg	-	-	-	-	-	-		+	
Pb	-	-	-	-	-	-	-		+
Ra	-	-	-	-	-	-			

3.7. Predicting New Compounds of Composition $A^{II}B^{III}F_5$ with Crystal Structure Types of $BaFeF_5$, $BaGaF_5$, $CaCrF_5$, $CaFeF_5$, $SrFeF_5$, and etc.

Phases with composition ABF_5 are of interest for search of compounds which hold promise for new ferro-electrics and materials for laser matrices [24]. We attempted to predict the new compounds of this composition with the crystal structure type of $BaFeF_5$ (space group P4, Z=32) [39,40], $BaGaF_5$ (space group P2(1)2(1)2(1), Z=4) [40,41], $CaCrF_5$ (space group P2(1)/c, Z=4) [39,40,42,43], $CaFeF_5$ (space group C222, Z=16) [40,43], and $SrFeF_5$ (space group P2(1)/c, Z=8) [40]. The crystal types with acentric space groups ($BaFeF_5$, $BaGaF_5$, and $CaFeF_5$) are of the greatest interest for search for new electro-optical, ferro-electric, and other materials for new technologies.

3.7.1. Data for Computer Learning

The data for computer learning was extracted from the DB on ternary inorganic compound properties [18-21]. Table 3.7.1 contains a resulting learning set.

Table 3.7.1
Learning Set for Predicting Crystal Structure Types
of Compounds with Composition ABF_5

Composition	Crystal type	Space group
SrAlF5	BaFeF5	
EuAlF5	BaFeF5	
PbAlF5	BaFeF5	
BaTiF5	BaFeF5	
BaVF5	BaFeF5	
SrCrF5	BaFeF5	
BaFeF5	BaFeF5	
SrGaF5	BaFeF5	
PbGaF5	BaFeF5	
BaTlF5	BaFeF5	
BaAlF5	BaGaF5	
BaCrF5	BaGaF5	
BaMnF5	BaGaF5	
SrNiF5	BaGaF5	
BaGaF5	BaGaF5	
CaTiF5	CaCrF5	
CaVF5	æaCrF5	
CaCrF5	CaCrF5	
CaCoF5	CaCrF5	
CaGaF5	CaCrF5	
CdCoF5	CaCrF5	
CaFeF5	CaFeF5	
CdCrF5	CaFeF5	
CdGaF5	CaFeF5	
SrTiF5	SrFeF5	
SrVF5	SrFeF5	
SrFeF5	SrFeF5	

Composition	Crystal type	Space group
SrCoF5	SrFeF5	
BaInF5	SrFeF5	
MnAlF5		Cmcm, Z=2
MnGaF5	MnGrF5	Cmmm, Z=8
BaCoF5	alfa-BaTiOF4	Pca2(1) (Pbcm), Z=4
CuAuF5	CuAuF5	P1(-), Z=1
AgAuF5	CuAuF5	P1(-), Z=1
SrSbF5		Pbcm, Z=4
BaSbF5		Pbcm, Z=4
CaAlF5		rhombic, Z=8
CrAlF5		monoclinic, Z=4
TiCrF5		monoclinic, Z=4
VCrF5		monoclinic, Z=4
TiPF5		
CaMnF5		P2/c, Z=4
CaYF5		
CrMnF5		cubic
		C2/c, Z=4
		Cmmm, Z=8
SrMnF5		
CdMnF5		P2(1)/n, Z=4
MnInF5		
MnLuF5		
PbMnF5		P2(1)/c, Z=4
FeLuF5		
NiInF5		
BaNiF5		C222(1), Z=4
CuInF5		
ZnInF5		
SrRhF5		
BaYbF5		
FeFeF5		
CrCrF5		

Pseudo-Binary Systems in which Compound of Composition ABF_5 does not Form

MgF2-AlF3	without compound ABF5
MgF2-YF3	without compound ABF5
MgF2-LaF3	without compound ABF5
MgF2-CeF3	without compound ABF5
MgF2-PrF3	without compound ABF5
MgF2-NdF3	without compound ABF5
MgF2-SmF3	without compound ABF5
MgF2-EuF3	without compound ABF5
MgF2-GdF3	without compound ABF5
MgF2-TbF3	without compound ABF5

Composition	Crystal type	Space group
MgF2-DyF3	without compound ABF5	
MgF2-HoF3	without compound ABF5	
MgF2-ErF3	without compound ABF5	
MgF2-TmF3	without compound ABF5	
MgF2-YbF3	without compound ABF5	
MgF2-LuF3	without compound ABF5	
CaF2-ScF3	without compound ABF5	
CaF2-InF3	without compound ABF5	
CaF2-CeF3	without compound ABF5	
CaF2-PrF3	without compound ABF5	
CaF2-NdF3	without compound ABF5	
CaF2-SmF3	without compound ABF5	
CaF2-GdF3	without compound ABF5	
CaF2-TbF3	without compound ABF5	
CaF2-DyF3	without compound ABF5	
CaF2-HoF3	without compound ABF5	
CaF2-ErF3	without compound ABF5	
CaF2-TmF3	without compound ABF5	
CaF2-YbF3	without compound ABF5	
CaF2-LuF3	without compound ABF5	
CdF2-ScF3	without compound ABF5	
PbF2-ScF3	without compound ABF5	
MnF2-YF3	without compound ABF5	
MnF2-LaF3	without compound ABF5	
MnF2-CeF3	without compound ABF5	
MnF2-PrF3	without compound ABF5	
MnF2-NdF3	without compound ABF5	
MnF2-SmF3	without compound ABF5	
MnF2-GdF3	without compound ABF5	
MnF2-TbF3	without compound ABF5	
MnF2-DyF3	without compound ABF5	
MnF2-HoF3	without compound ABF5	
MnF2-ErF3	without compound ABF5	
MnF2-YbF3	without compound ABF5	
FeF2-NdF3	without compound ABF5	
FeF2-SmF3	without compound ABF5	
FeF2-GdF3	without compound ABF5	
FeF2-HoF3	without compound ABF5	
CoF2-GdF3	without compound ABF5	
CoF2-GdF3	without compound ABF5	
CoF2-GdF3	without compound ABF5	
CoF2-TbF3	without compound ABF5	
CoF2-DyF3	without compound ABF5	
CoF2-HoF3	without compound ABF5	
CoF2-ErF3	without compound ABF5	
CoF2-TmF3	without compound ABF5	
SrF2-YF3	without compound ABF5	
SrF2-LaF3	without compound ABF5	

Composition	Crystal type	Space group
SrF2-CeF3	without compound ABF5	
SrF2-PrF3	without compound ABF5	
SrF2-NdF3	without compound ABF5	
SrF2-SmF3	without compound ABF5	
SrF2-GdF3	without compound ABF5	
SrF2-TbF3	without compound ABF5	
SrF2-DyF3	without compound ABF5	
SrF2-HoF3	without compound ABF5	
SrF2-ErF3	without compound ABF5	
SrF2-TmF3	without compound ABF5	
SrF2-YbF3	without compound ABF5	
SrF2-LuF3	without compound ABF5	
CdF2-YF3	without compound ABF5	
PbF2-YF3	without compound ABF5	
BaF2-LaF3	without compound ABF5	
BaF2-CeF3	without compound ABF5	
BaF2-PrF3	without compound ABF5	
BaF2-NdF3	without compound ABF5	
BaF2-PmF3	without compound ABF5	
BaF2-SmF3	without compound ABF5	
BaF2-EuF3	without compound ABF5	
BaF2-TbF3	without compound ABF5	
BaF2-DyF3	without compound ABF5	
BaF2-HoF3	without compound ABF5	
BaF2-UF3	without compound ABF5	
EuF2-LaF3	without compound ABF5	
PbF2-SmF3	without compound ABF5	
EuF2-GdF3	without compound ABF5	
PbF2-HoF3	without compound ABF5	
PbF2-YbF3	without compound ABF5	

At first we predicted the possibility of forming compounds of composition ABF_5 (divided into two classes - dichotomy). Next, we predicted the above-mentioned crystal types at standard conditions (at room temperature and normal pressure) for predicted on the first stage compounds (multiclass predicting).

3.7.2. Selection of Features

On the basis of physical-chemical grounds three sets of constituent component features were selected for the description of fluoride systems and compounds.

The first feature set coincides with Set V (see Section 3.6.2).

The second feature set coincides with Set IV (see Section 3.5.1.2.2).

The third set of properties of simple fluorides (Feature Set VII) includes the following information: the temperatures of melting for simple fluorides, their standard entropies at 298 K, and standard enthalpy of formation for corresponding simple fluorides, the ionic radii of the corresponding cations of elements A and B (Table 3.7.2). The properties were quantized on the basis of the uniform distribution of the interval values.

Table 3.7.2
Gradations for Feature Set VII
(Properties of Simple Fluorides)

Feature	Gradation	Feature	Gradation
Melting point of fluorides, K		Standard enthalpy of formation for corresponding simple fluorides, kcal/mol	
[10-292]	TM1	[2-64.2]	H1
(292-338]	TM2	(64.2-122]	H2
(338-403]	TM3	(122-140]	H3
(403-660]	TM4	(140-162.5]	H4
(660-830]	TM5	(162.5-190]	H5
(830-990]	TM6	(190-220]	H6
(990-1100]	TM7	(220-237]	H7
(1100-1210]	TM8	(237-260]	H8
(1210-1268]	TM9	(260-287]	H9
(1268-1350]	TM10	(287-330]	H10
(1350-1430]	TM11	(330-361]	H11
(1430-1510]	TM12	(361-395]	H12
(1510-1593]	TM13	(395-411.7]	H13
(1593-1673]	TM14	(411.7-455]	H14
(1673-1825]	TM15	(455-525.13]	H15
Standard entropy for corresponding simple fluorides, cal/mol*K		Ionic radii, A	
[1-17.5]	S1	[0-0.47]	R1
(17.5-19.8]	S2	(0.47-0.64]	R2
(19.8-21.5]	S3	(0.64-0.67]	R3
(21.5-25]	S4	(0.67-0.73]	R4
(25-26.6]	S5	(0.73-0.78]	R5
(26.6-27.54]	S6	(0.78-0.83]	R6
(27.54-28.5]	S7	(0.83-0.87]	R7
(28.5-30.14]	S8	(0.87-0.90]	R8
(30.14-35.19]	S9	(0.90-0.97]	R9
(35.19-37.5]	S10	(0.97-1.02]	R10
(37.5-43.3]	S11	(1.02-1.13]	R11
(43.3-54.75]	S12	(1.13-1.65]	R12
(54.75-68]	S13		
(68-80]	S14		

3.7.3. Prediction of Formation

In the case of predicting the formation of the compounds with composition ABF_5 the computer learning is carried out for three learning sets in which the compounds from Table 3.7.1 were described in terms of the sets of the component properties VI, V, and VII. The system of concept formation CONFOR [14] was used for computer learning and prediction.

3.7.4. Prediction of Crystal Structure

In the case of predicting the crystal structure type of the compounds with composition ABF_5 the computer learning is carried out for three learning sets in which the compounds from Table 3.7.1 were described in terms of the sets of the component properties VI, V, and VII also. The system of concept formation CONFOR [14] was used for computer learning and prediction also.

The pyramidal networks and the corresponding logical expressions were formed as a result of the computer learning via CONFOR. Appendix 5 contains the logical expressions for various learning sets for case of the prediction of crystal type.

The table of predictions of the crystal structure type for the compounds of composition ABF_5 (Table 3.7.3) results from comparison of the results of predicting possibility of formation and crystal structure type with use of the descriptions in terms of the Features Sets IV, V, VII (see Section 2.6.3). The following designations are used:

B - $BaFeF_5$;
G - $BaGaF_5$;
C - $CaCrF_5$;
F - $CaFeF_5$;
S - $SrFeF_5$;
\- - the crystal structure differing from those listed above;
? - the compound of composition ABF_5 exists but its structure type did not be predicted;
* - the compound of composition ABF_5 does not form.

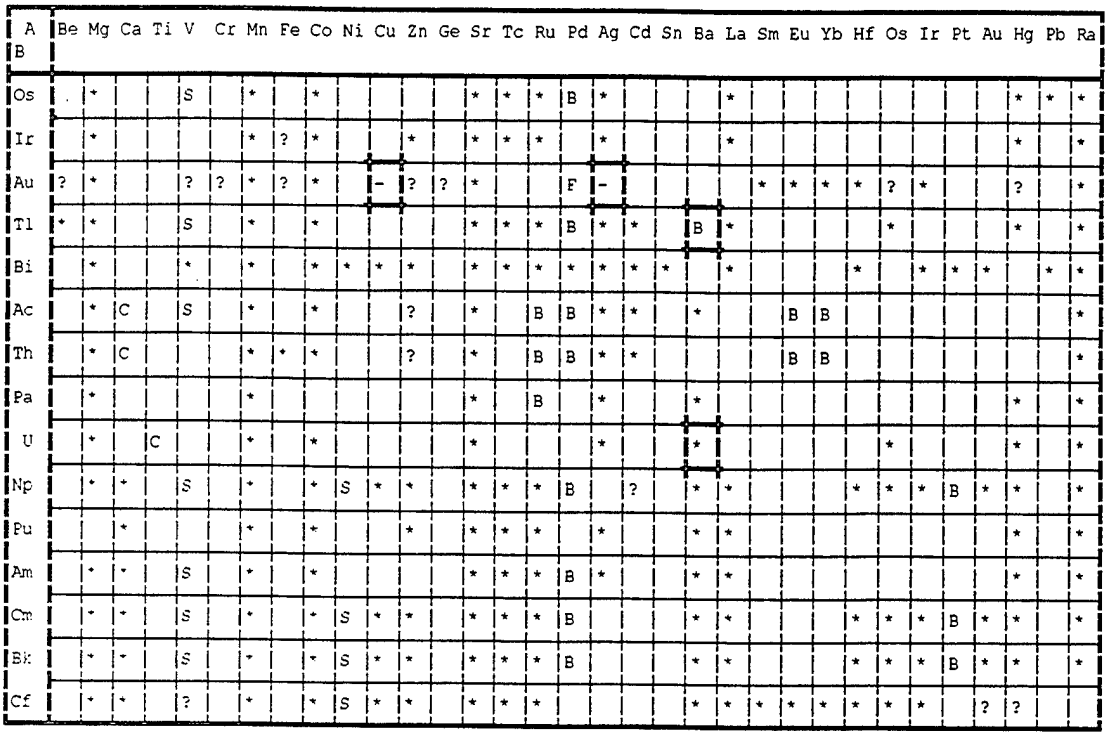
The physical-chemical systems, which were investigated experimentally, were outlined by double lines. The empty square corresponds to the lack of coincidence of the predictions, which have been obtained using different feature sets.

The analysis of Table 3.7.3 shows: the great number of predictions of new compounds with crystal structure type of $BaFeF_5$ and $CaFeF_5$, which hold the promise for searching for new electro-optical materials, were obtained.

Table 3.7.3
Table of Predictions of the Crystal Structure Type
for Compounds of Composition A(II)B(III)F_5

A / B	Be	Mg	Ca	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ge	Sr	Tc	Ru	Pd	Ag	Cd	Sn	Ba	La	Sm	Eu	Yb	Hf	Os	Ir	Pt	Au	Hg	Pb	Ra
B								*			?		*		?	B	*					B				B							
Al		*	F			-	G			C	G	G	B	?	?			?	?	G		B	B		B		B		?	G	B	G
P													*			B	*		-		*		*	*						*		*
Sc			*							G			*		?		*	*		*					B		B	B		*	*	*
Ti	?		C		?		C		C	-	?	?	S	F	?	?				B		C				C			-	B		B
V	B		C	?						B	B	F	S	F	?					B					S	B		?	B	?	B
Cr	C		C						?	C	?		B		?			F	F	G								?	?		B
Mn				C			F				F				?		*	F		G		B							-	G		
Fe	F		F	?					F	F	F		S				*		F	B			*	*		F		?	B		B
Co	C		C				C						S			C	*	C		-	*		*	*						*	
Ni	?		F	C	S	?		?	?		?	?	?	G	F	?	S			F	S				S	S	?	?	?	?	?	?
Ga	C		C	?	C	C	-	C			?	C		B	G			*	F		G									C	B	

A / B	Be	Mg	Ca	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ge	Sr	Tc	Ru	Pd	Ag	Cd	Sn	Ba	La	Sm	Eu	Yb	Hf	Os	Ir	Pt	Au	Hg	Pb	Ra
As					S									*	*	*	B	*				*		*	*						*		*
Y		*				*	*						*	*	*	*	*	*	*	*		*		*	*	*	*	*			*		
Ru	?					?								*	*			*	*			*		*	*						*	*	*
Rh															*	B		*	F			*		*	*								
In			*		?				?	-	?		*					*			S	*	*	*	*	*		*			?		
Sb	?				?		*							-	*	*		*			-												
La		*					*		*					*	*	*		*	*		*			*							*	*	*
Ce		*	*				*		*	*				*	*	*		*	*		*								B			*	
Pr		*	*				*	*	*	*			*	*	*	*		*	*		*								B			*	
Nd		*	*			*	*	*	*	*			*	*	*	*		*	*		*	*		*	*							*	*	*
Pm			*		?		*		*		-	?	?	*	*	*		*	*		*	*		*	*								*
Sm	*	*	*				*	*	*		*			*	*	*		*	*	*	*	*		*	*	*	*	*	*	*	*	*	*	*
Eu	*	*	*				*		*		*			*	*	*		*	*	*	*	*	*		*	*	*	*	*	*	*	*	*	*
Gd		*	*				*	*	*	*	*		*	*				*	*	*	*		*	*	*	*		*	*	*	*	*	*	*
Tb		*	*				*		*				*	*	*	*		*	*		*								B		*	*	*
Dy		*	*				*	*	*	*				*	*	*		*	*		*								B			*	
Ho		*	*				*	*	*	*				*	*	*		*	*		*								B			*	
Er		*	*				*	*	*	*				*	*	*		*	*		*								B			*	
Tm		*	*				*		*	*			*	*				*	*		*	B				B		B	B			*	
Yb		*	*				*		*	*			*	*	*	*		*	*										B			*	
Lu		*	*						*					*				*					B	B	B	B		B	B			*	*



A / B	Be	Mg	Ca	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ge	Sr	Tc	Ru	Pd	Ag	Cd	Sn	Ba	La	Sm	Eu	Yb	Hf	Os	Ir	Pt	Au	Hg	Pb	Ra
Os	.	*			S		*		*					*	*	*	B	*				*								*	*	*
Ir		*					*	?	*			*		*	*	*		*				*								*		*
Au	?	*			?	?	*	?	*		-	?	?	*			F	-				*	*	*	*	?	*			?		*
Tl	*	*			S		*		*					*	*	*	B	*	*		B	*				*				*		*
Bi		*			*		*		*	*	*	*		*	*	*	*	*	*	*		*			*		*	*	*		*	*
Ac		*	C		S		*		*			?		*		B	B	*	*		*			B	B							*
Th		*	C				*	*	*			?		*		B	B	*	*					B	B							*
Pa		*					*							*		B		*			*									*		*
U		*		C			*		*					*				*			*						*			*		*
Np		*	*		S		*		*	S	*	*		*	*	*	B		?		*	*				*	*	*	B	*	*		*
Pu			*				*		*			*		*	*	*		*			*	*								*		*
Am		*	*		S		*		*					*	*	*	B	*			*	*								*		*
Cm		*	*		S		*		*	S	*	*		*	*	*	B				*	*				*	*	*	B	*	*		*
Bk		*	*		S		*		*	S	*	*		*	*	*	B				*	*				*	*	*	B	*	*		*
Cf		*	*		?		*		*	S	*	*		*	*	*					*	*	*	*	*	*	*	*		?	?		

3.8. Predicting Crystal Structure Types of Compounds with Composition A_2BF_6

3.8.1. Predicting New Compounds of Composition $A^{I}{}_2B^{IV}F_6$ with Crystal Structure Types of Na_2SiF_6, K_2PtCl_6, K_2GeF_6-II, K_2MnF_6-II, K_2ZrF_6, beta1-K_2UF_6, trirutile, and etc.

Phases with composition A_2BF_6 are of interest for search for compounds which hold promise for new ferro-electrics and electro-optical materials [24]. We attempted to predict the new compounds of this composition with the crystal structure type of Na_2SiF_6 (space group P321, Z=3) [40, 44], K_2PtCl_6 (space group Fm3m, Z=4) [45], K_2GeF_6-II (space group P3(-)m1, Z=3) [40,45], K_2MnF_6-II (space group P6(3)mc, Z= 2), K_2ZrF_6(space group Cmcm, Z=4) [40,45,46], beta1-K_2UF_6 (space group P6(-)2m, Z=1) [40,45,46], and trirutile (space group P4(2)/mnm, Z=2) [40]. The crystal types with acentric space groups (Na_2SiF_6 and beta1-K_2UF_6) are of the greatest interest for search for new electro-optical, ferro-electric, and other materials for electronics.

3.8.1.1. Data for Computer Learning

The data for computer learning was extracted from the DB on ternary inorganic compound properties [18-21]. Table 3.8.1.1 contains a resulting learning set.

Table 3.8.1.1
Learning Set for Predicting Crystal Structure Types
of Compounds with Composition $A^{I}_{2}B^{IV}F_{6}$

Composition	Crystal type	Space group
H2SiF6		
H2GeF6		
H2PtF6		
Na2ZrF6		
Na2TcF6		
Na2HfF6		
Cu2SiF6		
K2FeF6		
K2MoF6		
K2PuF6		
Cs2TcF6		
Cs2TbF6		
Cs2ThF6		
Tl2ThF6		
Li2SiF6	Na2SiF6	
Li2MnF6	Na2SiF6	
Na2SiF6	Na2SiF6	
Na2TiF6	Na2SiF6	
Na2CrF6	Na2SiF6	
Na2MnF6	Na2SiF6	
Na2GeF6	Na2SiF6	
Na2RuF6	Na2SiF6	
Na2PdF6	Na2SiF6	
Na2OsF6	Na2SiF6	
Na2IrF6	Na2SiF6	
Na2PtF6	Na2SiF6	
Na2ThF6	Na2SiF6	
Na2UF6	Na2SiF6	
Na2NpF6	Na2SiF6	
Na2PuF6	Na2SiF6	
Li2TiF6	trirutile	
Li2VF6	trirutile	
Li2CrF6	trirutile	
Li2GeF6	trirutile	
Li2PdF6	trirutile	
Li2MoF6	trirutile	
Li2PtF6	trirutile	
Na2MoF6	trirutile	
Na2SnF6	trirutile	
Na2ReF6	trirutile	
Na2PbF6	trirutile	
Li2ZrF6	K2GeF6-II	
Li2SnF6	K2GeF6-II	
Li2HfF6	K2GeF6-II	
Li2PbF6	K2GeF6-II	

Composition	Crystal type	Space group
K2GeF6	K2GeF6-II	
K2TcF6	K2GeF6-II	
K2RuF6	K2GeF6-II	
K2PdF6	K2GeF6-II	
K2SnF6	K2GeF6-II	
K2ReF6	K2GeF6-II	
K2OsF6	K2GeF6-II	
K2IrF6	K2GeF6-II	
K2PtF6	K2GeF6-II	
K2PbF6	K2GeF6-II	
Rb2TiF6	K2GeF6-II	
Cs2TiF6	K2GeF6-II	
Tl2TiF6	K2GeF6-II	
Tl2GeF6	K2GeF6-II	
Rb2ZrF6	K2GeF6-II	
Rb2TcF6	K2GeF6-II	
Rb2SnF6	K2GeF6-II	
Rb2HfF6	K2GeF6-II	
Rb2ReF6	K2GeF6-II	
Rb2IrF6	K2GeF6-II	
Rb2PtF6	K2GeF6-II	
Rb2PbF6	K2GeF6-II	
Cs2ZrF6	K2GeF6-II	
Cs2RuF6	K2GeF6-II	
Cs2SnF6	K2GeF6-II	
Cs2HfF6	K2GeF6-II	
Cs2ReF6	K2GeF6-II	
Cs2OsF6	K2GeF6-II	
Cs2IrF6	K2GeF6-II	
Cs2PtF6	K2GeF6-II	
Cs2PbF6	K2GeF6-II	
Na2CeF6	beta1-K2UF6	
K2CeF6	beta1-K2UF6	
K2ThF6	beta1-K2UF6	
K2UF6	beta1-K2UF6	
K2NpF6	beta1-K2UF6	
Rb2CeF6	beta1-K2UF6	
Rb2ThF6	beta1-K2UF6	
Cs2CeF6	beta1-K2UF6	
K2SiF6	K2PtCl6	
Rb2SiF6	K2PtCl6	
Cs2SiF6	K2PtCl6	
Tl2SiF6	K2PtCl6	

Composition	Crystal type	Space group
K2TiF6	K2PtCl6	
K2CrF6	K2PtCl6	
Rb2CrF6	K2PtCl6	
Cs2CrF6	K2PtCl6	
Cs2MnF6	K2PtCl6	
Rb2GeF6	K2PtCl6	
Cs2GeF6	K2PtCl6	
Rb2RuF6	K2PtCl6	
Rb2PdF6	K2PtCl6	
Cs2PdF6	K2PtCl6	
K2VF6	K2MnF6-II	
K2MnF6	K2MnF6-II	
Rb2VF6	K2MnF6-II	
Rb2MnF6	K2MnF6-II	
K2ZrF6	K2ZrF6	
K2TbF6	K2ZrF6	
K2HfF6	K2ZrF6	
Rb2TbF6	K2ZrF6	
Rb2UF6	K2ZrF6	
Rb2NpF6	K2ZrF6	
Rb2PuF6	K2ZrF6	
Cs2UF6	K2ZrF6	
Cs2PuF6	K2ZrF6	
Tl2UF6	K2ZrF6	
Tl2NpF6	K2ZrF6	
Na2PrF6	gamma-Na2UF6	Immm, Z=2
Cs2VF6	RbNiCrF6	Fd3m, Z=8
Tl2ZrF6	(NH4)2ZrF6	Pmma, Z=8
Pseudo-Binary Systems in which Compound of Composition A_2BF_6 does not Form		
LiF-ThF4	without compound AB2F6	
LiF-UF4	without compound AB2F6	

At first we predicted the possibility of forming compounds of composition $A^{I}{}_2B^{IV}F_6$ (divided into two classes - dichotomy). Next, we predicted the above-mentioned crystal types at standard conditions (at room temperature and normal pressure) for predicted on the first stage compounds (multiclass predicting).

3.8.1.2. Selection of Features

On the basis of physical-chemical grounds three sets of constituent component features were selected for the description of fluoride systems and compounds.

The first feature set coincides with Set V (see Section 3.6.2).

The second feature set coincides with Set IV (see Section 3.5.1.2.2).

The third feature set coincides with Set VII (properties of simple fluorides (see Section 3.7.2).

3.8.1.3. Prediction of Formation

In the case of predicting the formation of the compounds with composition $A^{I}_2B^{IV}F_6$ the computer learning is carried out for three learning set in which the compounds from Table 3.8.1.1 were described in terms of the sets of the component properties VI, V, and VII. The system of concept formation CONFOR [14] was used for computer learning and prediction.

3.8.1.4. Prediction of Crystal Structure

In the case of predicting the crystal structure type of the compounds with composition $A^{I}_2B^{IV}F_6$ the computer learning is carried out for three learning sets in which the compounds from Table 3.8.1.1 were described in terms of the sets of the component properties VI, V, and VII also. The system of concept formation CONFOR [14] was used for computer learning and prediction also.

The pyramidal networks and the corresponding logical expressions were formed as a result of the computer learning via CONFOR. Appendix 6 contains the logical expressions for various learning sets for case of the prediction of crystal type.

The table of predictions of the crystal structure type for the compounds of composition $A^{I}_2B^{IV}F_6$ (Table 3.8.1.2) results from comparison of the results of predicting possibility of formation and crystal structure type with use of the descriptions in terms of the Features Sets IV, V, VII (see Section 2.6.3). The following designations are used:

N - Na_2SiF_6;
R - trirutile;
K - K_2PtCl_6;
G - K_2GeF_6-II;
M - K_2MnF_6-II;
U - beta1-K_2UF_6;
Z - K_2ZrF_6;
? - the compound of composition A_2BF_6 exists but its structure type did not be predicted;
- - the crystal structure differing from those listed above;
* - the compound of composition A_2BF_6 does not form.

The physical-chemical systems, which were investigated experimentally, were outlined by double lines. The empty square corresponds to the lack of coincidence of the predictions, which have been obtained using different feature sets.

The analysis of Table 3.8.1.2 shows: the great number of predictions of new compounds with crystal structure type of K_2GeF_6-II and K_2ZrF_6 were obtained. New compounds with acentric space groups (crystal structure type of Na_2SiF_6, space group P321): Na_2VF_6 and Na_2PaF_6, and (crystal structure type of beta1-K_2UF_6, space group P6(-)2m): Cs_2TbF_6, Tl_2TbF_6, Cs_2NpF_6, Tl_2PuF_6, K_2AmF_6, Cs_2AmF_6, Cs_2CmF_6, Tl_2CmF_6, Rb_2BkF_6, Cs_2BkF_6, Tl_2BkF_6, Rb_2CfF_6, Cs_2CfF_6, and Tl_2CfF_6, which hold the promise for searching for new electro-optical materials, - were predicted also.

Table 3.8.1.2
Table of Predictions of the Crystal Structure Type
for Compounds of Composition $A^{I}_2B^{IV}F_6$

A / B	Li	Na	K	Rb	Cs	Tl
Si	N	N	K	K	K	K
Ti	R	N	K	G	G	G
V	R	N	M	M	-	
Cr	R	N	K	K	K	
Mn	N	N	M	M	K	
Fe		R	K	M	M	G
Co		R	K	M	K	G
Ni		K	K	K	K	G
Ge	R	N	G	K	K	G
Zr	G	R	Z	G	G	-
Nb	G	R	G			G
Mo	R	R	G		M	
Tc		R	G	G		
Ru		N	G	K	G	
Rh	R	N	G	G	M	G
Pd	R	N	G	K	K	
Sn	G	R	G	G	G	
La		?	G	G	G	

A / B	Li	Na	K	Rb	Cs	Tl
Ce		U	U	U	U	
Pr		-	U	G	G	
Tb		R	Z	Z	Z	Z
Hf	G	R	Z	G	G	
Ta		?	G	G	G	
W		?	G	G	G	
Re		R	G	G	G	
Os		N	G		G	
Ir		N	G	G	G	
Pt	R	N	G	G	G	
Pb	G	R	G	G	G	
Th	*	N	U	U	?	
Pa		N		G		
U	*	N	U	Z	Z	Z
Np		N	U	Z	Z	Z
Pu		N	U	Z	Z	Z
Am		?	Z	Z	Z	
Cm		?	U	Z	Z	Z
Bk		?	U	Z	Z	Z
Cf		?	U	Z	Z	Z

3.8.2. Predicting New Compounds of Composition $A^{II}_2B^{II}F_6$ with Crystal Structure Types of Ba_2MnF_6, Ba_2CuF_6, Pb_2ZnF_6, rutile, and etc.
Phases with composition A_2BF_6 (i.e., Ba_2ZnF_6 and Sr_2CuF_6) are of interest for compounds which hold promise for new ferro-electric and electro-optical materials [24]. We attempted to predict the new com-

pounds of this composition with the crystal structure type of Ba_2MnF_6 (space group I422, Z=2) [40,43], Ba_2CuF_6 (space group I2/m, Z=2) [40,43], Pb_2ZnF_6 (space group P4(2)/nbc, Z=8) [40], and rutile (space group P4(2)/mnm, Z=0.66) [40]. The crystal type with acentric space group (Ba_2MnF_6) is of the greatest interest for search for new electro-optical materials.

3.8.2.1. Data for Computer Learning

The data for computer learning was extracted from the DB on ternary inorganic compound properties [18-21]. Table 3.8.2.1 contains a resulting learning set.

Table 3.8.2.1
Learning Set for Predicting Crystal Structure Types of Compounds with Composition $A^{II}_2B^{II}F_6$

Composition	Crystal type	Space group
Mg2MnF6	rutile	
Mn2MgF6	rutile	
Mg2FeF6	rutile	
Fe2MgF6	rutile	
Ba2MgF6	Ba2MnF6	
Ba2MnF6	Ba2MnF6	
Ba2FeF6	Ba2MnF6	
Ba2CoF6	Ba2MnF6	
Ba2NiF6	Ba2MnF6	
Ba2ZnF6	Ba2MnF6	
Ba2CrF6	Ba2CuF6	
Ba2CuF6	Ba2CuF6	
Pb2CuF6	Ba2CuF6	
Pb2MnF6	Pb2ZnF6	
Pb2FeF6	Pb2ZnF6	
Pb2CoF6	Pb2ZnF6	
Pb2NiF6	Pb2ZnF6	
Pb2ZnF6	Pb2ZnF6	
Sn2SrF6		rhombic, Z=4
Cd2BaF6		C222(1), Z=8
Sn2BaF6		rhombic, Z=4

Pseudo-Binary Systems in which Compound of Composition A_2BF_6 does not Form

BeF2-MgF2	without compound AB2F6
BeF2-ZnF2	without compound AB2F6
BeF2-BaF2	without compound AB2F6
BeF2-PbF2	without compound AB2F6
CaF2-MgF2	without compound AB2F6
MgF2-CoF2	without compound AB2F6

Composition	Crystal type	Space group
MgF2-NiF2	without compound AB2F6	
MgF2-CdF2	without compound AB2F6	
CaF2-MnF2	without compound AB2F6	
CaF2-CoF2	without compound AB2F6	
CaF2-NiF2	without compound AB2F6	
CaF2-SrF2	without compound AB2F6	
CaF2-CdF2	without compound AB2F6	
CaF2-BaF2	without compound AB2F6	
CaF2-EuF2	without compound AB2F6	
CaF2-PbF2	without compound AB2F6	
MnF2-ZnF2	without compound AB2F6	
MnF2-SrF2	without compound AB2F6	
CoF2-NiF2	without compound AB2F6	
CoF2-SrF2	without compound AB2F6	
CoF2-CdF2	without compound AB2F6	
NiF2-SrF2	without compound AB2F6	
NiF2-CdF2	without compound AB2F6	
ZnF2-CdF2	without compound AB2F6	
SrF2-BaF2	without compound AB2F6	
SrF2-PbF2	without compound AB2F6	
CdF2-PbF2	without compound AB2F6	
SnF2-PbF2	without compound AB2F6	
BaF2-EuF2	without compound AB2F6	

At first we predicted the possibility of forming compounds of this (divided into two classes - dichotomy). Next, we predicted the above--mentioned crystal types at standard conditions (at room temperature and normal pressure) for predicted on the first stage compounds (multiclass predicting).

3.8.2.2. Selection of Features

On the basis of physical-chemical grounds three sets of constituent component features were selected for the description of fluoride systems and compounds.

The first feature set coincides with Set V (see Section 3.6.2).

The second feature set coincides with Set IV (see Section 3.5.1.2.2).

The third feature set coincides with Set VII (properties of simple fluorides (see Section 3.7.2).

3.8.2.3. Prediction of Formation

In the case of predicting the formation of the compounds with composition $A^{II}_2B^{II}F_6$ the computer learning is carried out for three learning sets in which the compounds from Table 3.8.2.1 were described in terms of the sets of the component properties VI, V, and VII. The system of concept formation CONFOR [14] was used for computer learning and prediction.

3.8.2.4. Analyse of Semantic Networks and Corresponding Logical Expressions

Table 3.8.2.2 contains the results of analyse for various classes and for description of elements A^{II} and B^{II} in terms of feature set IV.

Table 3.8.2.2
Result of Analyse of Pyramidal Network (Feature Set IV)

Conjunction	Number of recurrences
Class of compound with composition A_2BF_6	19
R10, TD2	19
S, B2	17
C7, S8, H3	16
R10, TD2, C7, S8, H3	16
S, B2, E2	16
S, B2, E2, TM4	15
Without compound A_2BF_6	
S, B2	27
S, B2, E2	17
S, B2, E2, TM4	14
S, B2, H4	14
R10, TD2	13
R5, I17	12
I47, D, TD9	12
I47, D, TD9, I26	10
R9, E3	10
I12, I21	10

Analyse of Table 3.8.2.2 shows that the compounds with composition $A^{II}_2B^{II}F_6$ contain at least one element having standard capacity in the range from 26.377 to 27.18 kJ/kg*mol*K and entropy of individual substances at 298 K in the range between 59 and 69 kJ/kg*mol*K, and heat of melting in the range from 4.6 to 8.3 kJ/mol. A distinguishing characteristic of class "without compound A2BF6" is a presence in physico-chemical system at least one element with ionic radius in the range from 0.69 to 0.78 A and the first ionization potential in the

range from 7.432 to 7.87 eV, or d-element with the fourth ionization potential in the range from 52 to 56 eV and Debye temperature in the range from 405 to 465 K, and so forth. Conjunctions S & B2 and R10 & TD2 characterize all classes and don't be dividing.

Table 3.8.2.3 contains the results of analyse for various classes and for description of elements A^{II} and B^{II} in terms of feature set VII.

Table 3.8.2.3
Result of Analyse of Pyramidal Network (Feature Set VII)

Conjunction	Number of recurrences
Class of compound with composition A_2BF_6	
S1, H3	47
H3, S2	45
H3, S2, R12	45
S1, TM8	39
S1, H3, TM8	25
H3, S2, R12, TM6	25
S1, H3, TM9	24
S1, H3, R12, TM8	24
R12, S4	24
S1, H3, TM9, R10	23
H3, S2, R12, TM7	22
Without compound A_2BF_6	
TM11, H4	10
TM15, H10, R11	9
TM15, H10, R11, S1	9
TM11, H4, S2	9
TM11, H4, S2, R5	9

Analyse of Table 3.8.2.3 shows that the fields of compounds with composition $A^{II}{}_2B^{II}F_6$ and class "without compounds" of this composition don't intersect in the multidimensional space of feature set of simple fluorides. Thus this feature set is better for prediction of possibility of formation than previous one.

3.8.2.5. Prediction of Crystal Structure

In the case of predicting the crystal structure type of the compounds with composition $A^{II}{}_2B^{II}F_6$ the computer learning is carried out for three learning sets in which the compounds from Table 3.8.2.1 were described in terms of the sets of the component properties VI, V, and VII also. The system of concept formation CONFOR [14] was used for computer learning and prediction also.

The pyramidal networks and the corresponding logical expressions were formed as a result of the computer learning via CONFOR. Appendix 7 contains the logical expressions for various learning sets for case of the prediction of crystal type.

The table of predictions of the crystal structure type for the compounds of composition $A^{II}_2B^{II}F_6$ (Table 3.8.2.4) results from comparison of the results of predicting possibility of formation and crystal structure type with use of the descriptions in terms of the Features Sets IV, V, VII (see Section 2.6.3). The following designations are used:

B - Ba_2MnF_6;
R - rutile;
C - Ba_2CuF_6;
Z - Pb_2ZnF_6;
- - the crystal structure differing from those listed above;
? - the compound of composition A_2BF_6 exists but its structure type did not be predicted;
* - the compound of composition A_2BF_6 does not form.

The physical-chemical systems, which were investigated experimentally, were outlined by double lines. The empty square corresponds to the lack of coincidence of the predictions, which have been obtained using different feature sets.

The analysis of Table 3.8.2.4 shows: the great number of predictions of new compounds with acentric crystal structure type of Ba_2MnF_6 were obtained, which hold the promise for searching for new electro-optical materials.

Table 3.8.2.4
Table of Predictions of Crystal Structure Type
for Compounds of Composition $A^{II}_2B^{II}F_6$

A / B	Be	Mg	Ca	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Sr	Pd	Ag	Cd	Sn	Ba	La	Sm	Eu	Yb	Pt	Au	Hg	Pb	R
Be		*	*			*	*	*	*	*	*	*	*	*		*	*	*	*	*	B	B	*	*	*	*	
Mg	*		*			*	R	R	*	*	*		R			*		B									
Ca	*	*				*	*	*	*	*			*			*	*	*	*	*	*	*	*	*	*	*	*
Ti	*							R					*			*	*	B	?	?	?	?	C	*	*	*	
V	*							R					*			*	*	B	?	?	?	?	C	*	*	*	
Cr	*	*	*							R								C									C
Mn	*	R	*								*	*	*		*	*	*	B						*		Z	
Fe	*	R	*	R	R					R			*		R	*		B	B		B	B				Z	
Co	*	*	*							*	*	*	*			*	*	B						*		Z	
Ni	*	*	*			R		R	*		*	*	*			*	*	B						*		Z	
Cu	*	*					*		*	*					C			C	*		B	B				C	C
Zn	*						*		*	*			*			*	*	B	*	*			*	*		Z	
Sr	*	R	*	*	*		*	*	*	*		*			?		–	*	*		*	*			*	*	
Pd	*															*	*	B						*	*	*	
Ag							*	R			C		?					B		?			?	?	?	*	
Cd	*	*	*	*			*		*	*		*		*			*	–	*	*			*	*	*	*	–
Sn	*		*	*	*		*		*	*		*	–	*		*										*	*
Ba	*	B	*	B	B	C	B	B	B	B	C	B	*	B	B	–	–				*						

A / B	Be	Mg	Ca	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Sr	Pd	Ag	Cd	Sn	Ba	La	Sm	Eu	Yb	Pt	Au	Hg	Pb	R
La	*		*	?	?			B			*	*	*			*							C	*	*	*	
Sm	*		*	?	?							*			?	*					?	?	C			*	
Eu	B		*	?	?			B			B		*					*		?		?	C	?		*	
Yb	B		*	?	?			B			B		*							?	?		C	?		*	
Pt	*		*	C	C							*			?	*			C	C	C	C				*	
Au	*		*	*	*		*		*	*		*		*	?	*			*		?	?					
Hg	*		*	*	*								*	*	?				*								
Pb	*		*	*	*		Z	Z		Z	C	Z	*	*	*	*	*		*	*	*	*	*				
Ra			*			C					C				*	-											

3.9. Prediction of Type of Crystal Structure of Compounds with $A^{I}B^{V}O_3$ and $A^{II}B^{IV}O_3$ Compositions

The oxide compounds with ABO_3 composition is one of the most usefull classes of ferro-electric, electro-optical, non-linear optical, acousto-optical and other materials for electronics. It must be noted that perovskite-type cell, characteristic of the compounds with ABO_3 composition, is the basis of crystal structure of high-temperature superconductors. The class of ABO_3 compounds used in electronics contains apart from perovskites the compounds with different crystal structures (such as ilmenite, $LiNbO_3$, calcite, and so on) (Table 3.9.1).

Table 3.9.1

The compounds with ABO_3 composition used in electronics [24,47,48]

Composition	Crystal structure	Fields of use
$SrTiO_3$	perovskite, Pm3m	paraelectric, UHF-dielectric
$KTaO_3$	perovskite, Pm3m (or rhombically distorted perovskite)	paraelectric
$NaNbO_3$	ilmenite, R3(-) (or rhombically distorted perovskite (Pb2(1)m or P222(1)), or monoclinic distorted perovskite (mineral natroniobat))	UHF-dielectric

Composition	Crystal structure	Fields of use
$CaTiO_3$	rhombically distorted perovskite, Pbnm	UHF-dielectric
$LiNbO_3$	$LiNbO_3$, R3c	UHF-dielectric, piezo-electric for electro-mechanical converting signals and energy, industrial material for acousto--electronics, ferro-electric (T_C= 1200 æ), single crystals are used for the generation of the second harmonic in lasers and parametric light generation in infrared range, material for polarization optics (the value of birefringence = 0.09), acousto-optical, electro-optical and non-linear optical material
$LiTaO_3$	$LiNbO_3$, R3c	dielectric, piezo-electric, industrial material for acousto-electronics, pyroelectric, ferro-electric (Æß=655 æ), electro-optical material
$ZnTiO_3$	ilmenite, R3(-)	UHF-dielectric
$BaTiO_3$	tetragonally distorted perovskite, P4mm	piezo-electric for electro-mechanical converting signals and energy, ferro-electric (Æß= 130 æ), electro-optical material
$PbTiO_3$	tetragonally distorted perovskite, P4mm or P4/mmm	ferro-electric (Æß= 490 æ)
$KNbO_3$	hexagonally distorted perovskite (or rhombically distorted perovskite (Amm2))	ferro-electric (Æß= 435 æ), material for diode lasers
$CdTiO_3$	ilmenite, R3(-)	ferro-electric (Æß= -223 æ)
KNO_3	$KBrO_3$, R3m	ferro-electric (Æß= 124 æ)
$LiIO_3$	P4(1)	non-linear optical material, single crystals used for the generation of second harmonic in lasers and parametric light generation in infrared range

Composition	Crystal structure	Fields of use
$CaCO_3$	calcite, R3(-)c	material for polarization optics (the value of birefringence = 0.72)
$NaNO_3$	calcite , R3(-)c	material for polarization optics (the value of birefringence = 0.251)
$PbGeO_3$	alamosite ($PbSiO_3$), P2/n	acousto-optical material
$PbZrO_3$	rhombically distorted perovskite, Pbam	pyroelectric, ferro-electric

The analysis of experimental data [18,22-24] shows that the materials most useful in technology have crystal structures with restricted list of space groups. The most interesting electric and optical properties are exposed in the compounds belonged to 100 acentric space groups, but 80 % of all special properties been found are concentrated in 40 space groups, and 70% - in 9 selected space groups [24]. On one side it's caused by the fact that crystal structure defines many properties of a compound, on the other side - it is a consequence of a deliberate investigator's choice for synthesis and styduing of such compounds which isostructural with already known compounds with properties which are of interest to practical use. S.C.Abrahams made a great contribution to the development of theoretical methods of search for compound-analogs with special ferro-electric properties [49--51]. The main idea of his investigations completely coinsides with described above: a point group defines ferro-electric properties, that's why it is useful to look for the new compounds of this class among the analogs using the information of crystallographic databases (STN and other). However Abrahams could not predict new compounds of this class, having predicted only the properties for the compounds already known.

From our point of view the first step in prediction of new compounds with properties important for technics and depending upon the crystal structure is closely connected with prediction of possibility of formation of the compounds not yet synthesized, analogous to the compounds known already with special properties, and also with the prediction of their crystal structure type at normal condition and the possible distortion of ideal cell.

3.9.1. Attempts of Prediction of the Crystal Structures

The attempts to predict the type of crystal structure of compounds with ABO_3 composition have a long history. The most investigated one was the structure type of perovskite ($CaTiO_3$, space group Pm3m, Z=1). The idea about ions as incompressible balls forms the basis of a

classic description of crystal lattice of inorganic compounds. According to Goldschmidt the crystal structure and therefore the crystal type is determined by the number of structure units, the relationship of their dimensions and their polarization properties [52,53]. The structure unit should be understood as an atom or ion, or sometimes the group of atoms - molecule or complex ion.

In the context of the theory of close packing [54], the perovskite structure ($CaTiO_3$) appears, if the close packing is formed by oxygen ions and large-sized cations (Ca^{2+}), á 1/4 octahedral interstices is filled by small cations (Ti^{4+}). The theory of close packing lets us to find the geometrical conditions of existence of structures of perovskite, ilmenites and other. It's not hard to understand that the relationship of sizes of ions plays a dominant role in the appearance of these structures (from the point of view of the theory of close packing). In the case of perovskites with ABO_3 composition this circumstance was reflected in the tolerance factor advanced by Goldschmidt [53]:

$$t = \frac{R_A + R_O}{2^{1/2}\,(R_B + R_O)}, \qquad (1)$$

where R_A, R_B ¿ R_O - radii of corresponding cations and oxygen.

Goldschmidt [53] had found out, that for each of perovskites known at that time the tolerance factor lies in the range from 0.8 to 1.0. If the tolerance factor less than 0.8, the structure tranforms into the structure of another type, for example, ilmenite. For ilmenite structure (or corundum for the compounds with AAO_3 composition) the tolerance factor t lies in the range from 0.71 to 0.80.

Zachariasen [55] made two corrections to the expression (1). Multiplier 1.06 in numerator made it possible to consider the extension of a distance A-O with coordination number 12, and multiplier 0.95 in denominator - the restriction of distance B-O in octahedras BO_6.

These corrections restricted the tolerance factor for perovskites with the bounds of 0.9 - 1.1 [55]. However later it was shown by Naray-Szabo [56] that it's not useful to introduce the second correction into Zachariasen formula, that's why it's not taken into account in some papers.

Smolenski ¿ Agranovskaya [57] tried to find out the limits of changing of tolerance factor for complicated perovskites. In this case the values of the tolerance factor for perovskites, calculated by mean ionic radii, are restricted in bounds of 0.80 - 1.05.

Ramadass examined [58] crystal-chemical particulares of complicated perovskites with ABO_3 composition and electric and magnetic properties connected with them. By his calculations the values of tolerance factor t for the structures close to perovskites, lie in ranges from 0.75 to 1.0. The ideal undistorted cubic perovskite structure is realised with t=1. For t<1 the rhombic distortion of perovskites take place and the structures with lower coordination numbers of cations A are formed. The symmetry of these structures may correspond to the space groups R3c, R3(-)m or R3(-). When t comes close to lower bound (0.75), the rhombic distortion of perovskite elementary cell takes place. In case of large cations A (t>1) polytypic phases ABO_3 appear, in which some octahedras BO_6 have common faces. Some compounds of ABO_3 composition have another types of structure: ilmenites (for $R_A << R_B$ and t<0.75) and defect structures like pyrochlore. Namely in pyrochlores t>1 the spontaneous ferro-electric distortion of cubic perovskite cell towards decreasing of symmetry through displacement of B-cations in BO_6 octahedra takes place.

Fukunaga ¿ Fujita tried to predict the perovskite structure depending on mean interatomic distance [59] calculated arrording to the formula (2):

$$V^{1/3} = 2(mR_B + nR_O) - d(s-1), \qquad (2)$$

where m, n and d - some coefficients which, for example, equal 1.185, 0.882 for the compounds with $A^{2+}B^{4+}O_3$ composition correspondingly, s - opposite tolerance factor:

$$s = 2^{1/2}\,\frac{R_B + R_O}{R_A + R_O}\,.$$

Linear $V^{1/3}$ - dependence on s was found also for perovskites with ABF_3 and $ABCl_3$ composition.

The model of invariant distances by Poix [60,61] is based on the principle that cation always defined by the unchanged distance anion-cation, which value depends only upon the coordination number and valency and does not depend upon the structure of crystal. Poix advanced his variant of equation for the tolerance factor for combined perovskites [61]:

$$t = 1 - 1.707T,$$

where $T = 1 - A/2B$, $A = R_A + R_O$ and $B = R_B + R_O$ - invariant distances. According to the opinion [62], the Poix-model seems to be very fruitful for searching of the bounds of phase transition for oxide perovskites and calculation of lattice parameter for cubic perovskites of this composition.

Some other approach for finding geometrical conditions of existence was suggested by Wainer and Wentworth [63]. Apart from the limits of value of factor t (in form of Zachariasen [55]) they considered the tendency of cations to create the certain oxygen environment. The stable octahedral environment of ions B is possible for R_B/R_O lying in bounds of 0.41 - 0.73, cations A have oxygen environment with coordination number more then 6 for $R_A/R_O > 0.73$ [52]. Regarding this conditions it's possible to find ionic radii of cations, such that the compounds of ABO_3 composition have perovskite structure: R_A must lies in bounds of 1.00 - 1.69 A, R_B - in bounds of 0.57 - 1.02 A. However how it was shown by experiment these bounds do not always correspond to the real values of the existence of perovskite structure.

There is another approach for finding geometrical conditions of existence of types of crystal structure [64-67]. It was found out during the analysis of diagram of dependence of ion A radius on ion B radius that points, corresponding ABO_3 composition with different crystal structures cluster in separate domains. The boundary lines between the domains may be taken as geometrical conditions of existence of the compounds with particular structure type. However in this case the boundary values change greatly during the transition from one system of ionic radii to another. While building of such a structure field map (SFM) using the system of ionic radii Ahrens [68] the geometrical conditions of existence of perovskite structure are described by the following expressions [4]:

$$R_A > \text{or} = 0.90 \text{ A} \qquad (3)$$

$$0.51 \text{ A} < \text{or} = R_B < \text{or} = 1.10 \text{ A} \qquad (4)$$

$$R_A > R_B \qquad (5)$$

Condition (3) defines the stability of oxygen environment around cation with coordination number 12. Condition (4) is connected with stability of octachedral oxygen environment of cations B. The violation of condition (5) has a rezult that A and B ions change their places producing the inverse perovskite structure.

Fesenko, Filip`ev and Kupriyanov [4] choose the similar ways, examining SFM for complicated perovskites.

The close approach was introduced by Giaquinta and Zur Loye [69]. During the SFM building they took into account the electronegative of elements A and B, having the coordinate axes $(dX_{B-O})(R_B/R_O)$ - $- (dX_{A-O})(R_A/R_O)$, where dX - difference between electronegatives of element A or B and O. Using such SFM, the authors [69] found the sufficient successfull division of the domains of existence of the compounds with ABO_3 composition with perovskite, ilmenite and corundum structure types.

Goodenough and Kafalas made an attempt to consider several factors simultaneously during classification of perovskite-type compounds with $A_1+B_5+O_3$ composition [70]. They supposed that the bounds of stability of crystal modifications of these compounds are defined by the following factors: relative sizes of ions A and B, their elecrostatic interaction, polarizability of electronic shells of cations A, and part of covalence in B-O bond. The influence of all listed factors on the distortion of cubic cell of perovskite, determining the ferroelectric properties of corresponding compounds, was discussed in [70].

The type of t factor is not of great importance because different formula lead to small change of its value simultaneously for all compounds. It's important that starting bounds of change of tolerance factor for the perovskite-type compounds were calculated on the basis of restricted number of experimental data. The synthesis of new compounds with perovskite structure leads to reconsidering of the bounds of t-factor change. Many of new compounds with ilmenite structure are synthesized now for which the tolerance factor however has the values characteristic for the typical perovskite compounds.

So the tolerance factor lost it's importance for the classification. The new experimental data lead to the change (introduction a corrections, refinement) of the classification scheme and then to its failure.

Therefore if the approach to the problem discussed is solved using the position of the close packing theory, the type of crystal structure depends primarilly upon the ions sizes. According to this the problem is reduced to determination of the sizes of these ions. However this problem can't be solved with enough precision. The approximations given by the existing systems of effective ionic radii are correct for some set of compounds. The extrapolation to another fields leads sometimes to incorrect results. In this case it's nesessary to introduce corrections, connected with the change of the nature of interatomic bonds. The values of these corrections are defined by the distribution of electronic density, which in its turn depends upon the properties of elements involved in the reaction. Thus the correction for change of interatomic bond during the transition from one compound to another is the function of the properties of atoms forming the compound. In such a case:

$$z_{A'} = z_{A''} f(x_{1A}, x_{2A}, \ldots, x_{NA}, x_{1B}, x_{2B}, \ldots, x_{NB}),$$

where $z_{A'}$ and $z_{A''}$ - sizes of ion A in $A'_mB'_n$ and $A''_mB''_n$ compounds correspondingly; x_{iA} and x_{iB} ($i = 1, 2, \ldots, N$; N - the number of element's properties) - the properties of elements A ¿ B correspondingly.

It was precisely the fact considered by Goldschmidt [53], when he had pointed to the dependence of structure type upon the polarization properties of ions. The observed preference of some cations to fixed

coordination environments [71] serves as experimental confirmation of this fact. It's supposed [71] that the genesis of such a preference is twofold. From one side it is explained by partially covalent bond with use of hybridizated orbitals, from another side - by stabilisation in crystal field.

It may be noted analysing the information of DB Phases [18-21], concerning perovskites with ABO_3 composition, that compounds with perovskite structure been investigated until the present time have different types of symmetry: rhombic (59 % of the whole number of discovered perovskites), cubic (20 %), hexagonal (9 %), monoclinic (8 %) and tetragonal (4 %). These proportions change for different compositions of perovskites:

	rhombic	cubic	hexagonal	monoclinic	tetragonal	
$A^{I}B^{V}O_3$	23	50	10	13	4	%
$A^{II}B^{IV}O_3$	33	35	10	18	4	%
$A^{III}B^{III}O_3$	80	6	9	0	5	%

The perovskite cell of ABO_3 compounds with symmetry lower then cubic may be considered as distorted one, produced from the ideal by small deformations. Accounting the role of structure distortion for displaying electric and optical properties there were many attempts to predict the type of symmetry of perovskite-type compounds. The major difficulty while solving the facing problems is the contradictions of experimental data about the type of distorted lattice. There is no full unambiguity in solving the problem of lattice symmetry at fixed experiment conditions even for well-studied compounds.

Nevertheless some investigators tried to analyse experimental data in order to eleborate the cryteria of existence of different types of perovskite-type compounds.

Megaw [72] divided perovskites with two-valent ions into three groups in accordance with their symmetry: cubic with t lying in bounds 0.90 - 1.02, rhombic (with pseudo-monoclinic perovskite cell) with t in bounds of 0.80 - 0.90 and tetragonal with t in bounds of 0.97 - 1.02. Only geometrical factors were taken into account.

The geometrical approach to the classification of distorted perovskite cell, suggested by Yakel [73], proved to be unsuccessfull, that's why he had to consider another factors, determining the displacement of atoms and the symmetry of perovskite compounds. The covalence degree of chemical bonds was the first factor refered by Yakel to such a group of factors.

Naray-Szabo [74] apart from geometric sizes of ions considered also their polarizability. He divided perovskites into 4 groups - first two with small cations A (small polarizability) and two other with large cations A (strong polarizability):

1. Tolerance factor t is close to 1 and changes in bounds of 0.98 -

1.005. These are the ideal cubic perovskites.

2. t much differs from 1. These are the compounds with monoclinic (rhombic) structure and large unit cell, consisting of 8 perovskite cells.

3. t > 1.01. Compounds with small tetragonal cell (c/a > 1).

4. t < 1.01. Compounds with large tetragonal cell (in reality rhombic), consisting of 8 perovskite subcells (analogs of $PbZrO_3$).

Keith and Roy [75] tried to find the cryteria of existence of different structure types of ABO_3 compounds with three-valent elements. However the wrong separation of $YCrO_3$ analogs in original structure type, actually having monoclinic perovskite-type cell, depreciated the cryteria produced by them.

Wood [76] during the classification of compounds with ABO_3 composition proceeded from the main idea of Goldschmidt, that structure is defined for the most part by geometric factors, but he refused to use the tolerance factor t. Having built the SFM in coordinates R_A - R_B, the author managed to separate the partly intersecting fields with different symmetry: cubic, tetragonal, and rhombic. In order to take into account the phase transitions at different temperatures, the third coordinate axis was introduced - the temperature, which much complicated SFM, but have not lead to the increasing separateness.

Roth [77] have built the similar two-dimensional diagrams, but only separately for the compounds with compositions $A^{2+}B^{4+}O_3$ and $A^{3+}B^{3+}O_3$. These diagrams also displayed the partly intersection of fields of phase existence with different symmetry. That is why Roth built three-dimensional SFM, having chosen the porarizability of ion A^{2+} as a third axis. On this diagram it was possible to separate the fields of ferro-electrics and anti-ferro-electrics with easily polarizing ions A.

The main disadvantage of Wood and Roth diagrams is the small number of compounds used for their building. Fesenko, Filip`ev and Kupriyanov [4] tried to remove this disadvantage, making the field of the used examples more large, including perovskites of complicated composition. However SFM built in coordinates R_A - R_B, did not allow to make unambiguous classification of perovskite-type compounds according to symmetry types.

The classifying regularities, which consider only the sizes of cations and some other factors (i.e., polarizability, temperature and so on), do not separate well the perovskites from phases with another structure and much less do not allow to make more sophisticated classification of these compounds according to the types of distortion of ideal cubic cell. The whole history of searches for tolerance factor and its limits and also "good" two-dimensional diagrammes [52-77] - are the attempts to consider all new experimental data which do not accord the old scope. All the variants of such classification schemes created by a long and tedious work of investigators failed when the new experimental result contradicting the old classification appeared.

An ideal classification scheme must be adaptable construction, useful for recognizing any of new situations. The majority of empiric rules do not satisfy this demand. Many of corrections, caused by the storage of new experimental facts contradicting the old scheme, complicate these classification rules.

The problem of classification is to analyse the objects or phenomena, described by the set of properties. That's why it's natural to use the computers for the analysis of information, received by experiment or calculation. The use of high-speed computers lets us to classify practically any of experimental data array in multidimensional property spaces in a short time. All this gives the opportunity to make quick reexamination of classification schemes and regularities when new data appear.

The cybernetic prediction uses the methodology of computer learning for searching for classifying regularities. The main advantage of computer classification is the use of multidimensional dividing rules including not only ion sizes but also another components properties (thermochemical, energetic and so on). In order to find such regularities we have introduced the methods of the computer learning for inductive concept formation, intended for finding the complicated classification rules in multidimensional spaces of properties [14].

3.9.2. Predicting New Oxide Perovskites

The oxide perovskites were the first three-component phases, predicted by us about 25 years ago [78]. Since that time about 200 compounds with ÇéÄ$_3$ composition were synthesized, for half of them the crystal structure was investigated. The comparison of the predictions and experiment showed that reliability of prediction of new compounds with ÇéÄ$_3$ composition - 87 %, and their perovskite-type structure - - 77 %. These characteristics are good enough for the method of prediction of new phases based on "first principles". Five years ago we have tried also to predict the type of distortion of perovskite cell [37]. Unfortunatelly the number of new synthesized phases does not allow to estimate the reliability of our last predictions.

The analysis of a list of compounds with ABO$_3$ composition with special properties presented in Table 3.9.1, shows that it contains only the compounds with composition for two cations combination: $A^IB^VO_3$, and $A^{II}B^{IV}O_3$. These particular compositions have been chosen for prediction. The database on the properties of ternary compounds "Phases", developed in Institute of Metallurgy of RAS [18-21], contains the information on about 100 compounds with $Ç^Ié^VÄ_3$ composition and about 260 compounds with $A^{II}B^{IV}O_3$ composition and more than a half of them have perovskite-type structure.

On the first step using the methods of computer learning [14] it was made a search for regularities for the compounds with $A^{II}B^{IV}O_3$ compo-

sition, classifying oxide systems into two classes: with forming of compounds ÇéÄ3 and without forming of the compounds with such a composition at the normal conditions. 15 experimental examples of absence of compounds with composition ÇéÄ3 were used. The corresponding information was taken from the database "Phases" [18-21]. Then the type of crystal structure of new phases was predicted.

3.9.2.1. Predicting Crystal Structure Type of New Compounds with Composition $A^{I}B^{V}O_3$

3.9.2.1.1. Data for Computer Learning

For the compounds with $A^{I}B^{V}O_3$ composition only the type of crystal structure was predicted because in this case the DB "Phases" did not contain any example of absence of compounds with such a composition in physico-chemical systems. Table 3.9.2.1.1 contains a resulting learning set.

Table 3.9.2.1.1
Learning Set for Predicting Crystal Structure Types of Compounds with Composition $A^{I}B^{V}O_3$

Composition	Crystal type	Space group or symmetry
HNbO3	perovskite	cubic, rhombic
HTaO3	perovskite	cubic
NaCrO3	perovskite	cubic
NaNbO3	perovskite	hexagonal, monoclinic, rhombic (Pb2(1)m)
NaTaO3	perovskite	rhombic, monoclinic, cubic
NaWO3	perovskite	cubic
NaPaO3	perovskite	rhombic (GdFeO3-type)
NaUO3	perovskite	rhombic (GdFeO3-type), hexagonal
KNbO3	perovskite	hexagonal
KTaO3	perovskite	cubic, rhombic
KPaO3	perovskite	cubic
KUO3	perovskite	cubic
KNpO3	perovskite	?
RbIO3	perovskite	cubic
RbTaO3	perovskite	tetragonal, monoclinic
RbPaO3	perovskite	cubic
RbUO3	perovskite	cubic
AgNbO3	perovskite	cubic, rhombic, monoclinic
AgTaO3	perovskite	cubic, rhombic, monoclinic
CsIO3	perovskite	cubic
TlUO3	perovskite	cubic
LiNO3	calcite	R3(-)c
NaNO3	calcite	R3(-)c

Composition	Crystal type	Space group or symmetry
KNO3	aragonite	Pmcn, Z=4
LiNbO3	LiNbO3	R3c
LiTaO3	LiNbO3	R3c
LiUO3	LiNbO3	R3c
NaClO3	NaClO3	P2(1)3, Z=4
NaBrO3	NaClO3	P2(1)3, Z=4
NaIO3	NaClO3	P2(1)3, Z=4
NaBiO3	ilmenite	R3(-)
KSbO3	ilmenite	R3(-)
RbSbO3	ilmenite	R3(-)
AgSbO3	ilmenite	R3(-)
RbClO3	KBrO3	R3m
CsClO3	KBrO3	R3m
TlClO3	KBrO3	R3m
KBrO3	KBrO3	R3m
RbBrO3	KBrO3	R3m
CsBrO3	KBrO3	R3m
TlBrO3	KBrO3	R3m
TlIO3	KBrO3	R3m
LiPO3		P2/n, Z=8
HSbO3		cubic
HIO3		P2(1)2(1)2(1), Z=4
LiVO3	pyroxene	C2/c (Cc), Z=8
LiAsO3		C2/c, Z=8
LiBrO3		Pnma, Z=4
LiSbO3		Pncn, Z=4
LiIO3		P6(3), Z=2(32)
LiReO3		R3c
RbNO3		tetragonal, Z=4
AgNO3		Pbca (P222), Z=8
CsNO3		hexagonal
TlNO3		P2(1)2(1)2(1) (Pbnm), Z=4
NaPO3		P2(1)/n, Z=8
NaVO3	pyroxene	C2/c, Z=8
NaAsO3		P1(-), Z=6
NaSbO3	pyrochlore	Fd3m, Z=16
KPO3	KPO3(IV)	P2(1)/a, Z=8(4)
RbPO3		P2(1)/n, Z=4
AgPO3	AgPO3	P2(1)/n, Z=8
CsPO3		P2(1)/n, Z=4
TlPO3		P2(1)/n, Z=4
KClO3	KClO3	P2(1)/m, Z=2
AgClO3	AgClO3	I4/m (I4/mmm), Z=8

Composition	Crystal type	Space group or symmetry
KVO3	pyroxene	Pmab, Z=4
KIO3		P1, Z=4
KBiO3	beta-KSbO3	Pn3, Z=12
CuVO3		R3(-)
RbVO3	pyroxene	Pmab, Z=4
AgVO3		rhombic, Z=4
CsVO3	pyroxene	Pmab, Z=4
TlVO3	pyroxene	Pbcm, Z=4
CuNbO3		C2/m, Z=8
CuTaO3		R3(-)c
AgBrO3	AgClO3	I4/mmm, Z=8
RbNbO3		P1(-), Z=4
CsNbO3		P2(1)/c, Z=8
TlNbO3	pyrochlore	
AgIO3		Pcab (Pbc2(1), Z=8
TlTaO3	pyrochlore	cubic
		?
HNO3		?
HPO3		?
HClO3		?
HBrO3		?
HNpO3		?
LiClO3		?
LiPaO3		?
NaReO3		?
CuPO3		?
KAsO3		?
RbAsO3		?
CsAsO3		?
AgBiO3		?
AuSbO3		?
CsTaO3		?
CsPaO3		?
TlCrO3		?

We predicted the compounds with the crystal types of perovskite (ideal cell has space group Pm3m, Z=1) [45], aragonite (space group Pmcn, Z=4) [45], calcite (space group R3(-)c, Z=6 (hex.)) [45], $NaClO_3$ (space group P2(1)3, Z=4) [45], ilmenite (space group R3(-), Z=6 (hex.)) [45], $KBrO_3$ (space group R3m, Z=3 (trigon.)) [45], and $LiNbO_3$ (space group R3c, Z=6 (hex.)) [79,80] at standard conditions (at room temperature and normal pressure). The crystal types with acentric space groups ($KBrO_3$ and $LiNbO_3$) are of the greatest interest for search for new electro-optical, ferro-electric and other materials for electronics.

3.9.2.1.2. Selection of Features

On the basis of physical-chemical grounds three sets of constituent component features were selected for the description of oxide systems and compounds.

The first feature set coincides with Set V (see Section 3.6.2).

The second feature set coincides with Set IV (see Section 3.5.1.2.2).

The third set of properties of simple oxides (Feature Set VIII) includes the following information: the temperatures melting/decomposition for simple oxides, standard heat of formation for corresponding simple oxides, standard isobaric thermal capacities of simple oxides, the ionic radii of the corresponding cations, and formal valency of cations of elements A and B (Table 3.9.2.1.2). The properties were quantized on the basis of the uniform distribution of the interval values.

Table 3.9.2.1.2
Gradations for Feature Set VIII
(Properties of Simple Oxides)

Feature	Gradation	Feature	Gradation
Melting/decomposition point of oxides, K		Standard heat of formation for corresponding simple oxides, kcal/mol	
[10-400]	TM1	[-76.7-13.229]	H1
(400-700]	TM2	(13.229-48.5]	H2
(700-1000]	TM3	(48.5-62]	H3
(1000-1400]	TM4	(62-83.802]	H4
(1400-2000]	TM5	(83.802-103]	H5
(2000-2270]	TM6	(103-138.81]	H6
(2270-2660]	TM7	(138.81-151.79]	H7
(2660-3330]	TM8	(151.79-218.1]	H8
(1210-1268]	TM9	(218.1-260.3]	H9
Standard isobaric thermal capacity corresponding simple oxides at 298 K, cal/mol*K		(260.3-300]	H10
		(300-428]	H11
		(428-448.9]	H12
		(448.9-565]	H13
		Ionic radii, A	
[6.09-9.036]	C1	[0-0.35]	R1
(9.036-10.54]	C2	(0.35-0.57]	R2
(10.54-11.9]	C3	(0.57-0.64]	R3
(11.9-13.5]	C4	(0.64-0.67]	R4
(13.5-15.21]	C5	(0.67-0.72]	R5

Feature	Gradation	Feature	Gradation
(15.21-17.997]	C6	(0.72-0.80]	R6
(17.997-24.35]	C7	(0.80-0.85]	R7
(24.35-25.5]	C8	(0.85-0.89]	R8
(25.5-28.11]	C9	(0.89-0.97]	R9
(28.11-44.6]	C10	(0.97-1.01]	R10
Valency		(1.01-1.20]	R11
+1	V1	(1.20-1.74]	R12
+2	V2		
+3	V3		
+4	V4		
+5	V5		
+6	V6		
+7	V7		

3.9.2.1.3. Prediction of Crystal Structure

In the case of predicting the crystal structure type of the compounds with composition $A^{I}B^{V}O_3$ the computer learning is carried out for three learning sets in which the compounds from Table 3.9.2.1.1 were described in terms of the sets of the component properties VI, V, and VIII. The system of concept formation CONFOR [14] was used for computer learning and prediction.

The pyramidal networks and the corresponding logical expressions were formed as a result of the computer learning via CONFOR. Appendix 8 contains the logical expressions for various learning sets.

In the case of predicting the distortion of ideal cubic cell of perovskite for the compounds with composition $A^{I}B^{V}O_3$ the computer learning is carried out for each type of symmetry (cubic, monoclinic, rhombic, tetragonal, and hexagonal) and for three learning sets in which the compounds from Table 3.9.2.1.1 were described in terms of the sets of the component properties VI, V, and VIII.

The pyramidal networks and the corresponding logical expressions were formed as a result of the computer learning via CONFOR. Appendix 9 contains the logical expressions for various learning sets and for various types of symmetry.

The table of predictions of the crystal structure type for the compounds of composition $A^{I}B^{V}O_3$ (Table 3.9.2.1.3) results from comparison of the results of predicting the crystal structure type and distortion type with use of the descriptions in terms of the Features Sets IV, V, VIII (see Section 2.6.3). The following designations are used:

1 - cubic perovskite;
2 - rhombically distorted perovskite;
3 - hexagonally distorted perovskite;
4 - monoclinically distorted perovskite;
5 - tetragonally distorted perovskite;
P - perovskite with unknown symmetry;
C - calcite;
A - aragonite;
N - $NaClO_3$;
I - ilmenite;
K - $KBrO_3$;
L - $LiNbO_3$;
? - compound exists but it's crystal structure didn't be predicted;
- - the crystal structure differing from those listed above;
* - the compound of composition ABO_3 does not form.

The physical-chemical systems, which were investigated experimentally, were outlined by double lines. The empty square corresponds to the lack of coincidence of the predictions, which have been obtained using different feature sets.

The analysis of Table 3.9.2.1.3 shows: few new lithium compounds with crystal structure type $LiNbO_3$, which hold the promise for searching for new electro-optical materials, were obtained. The space group for $LiReO_3$ was obtained (R3c) [81] but its crystal type didn't be explaied. The fact of existence of compound $LiPaO_3$ without information about crystal structure was adduced in [82]. The crystal structure resembling $LiNbO_3$ was be predicted for these compounds.

Table 3.9.2.1.3
Table of Predictions of Crystal Structure Type
for Compounds of Composition $A^{I}B^{V}O_3$

A / B	H	Li	Na	K	Cu	Rb	Ag	Cs	Au	Tl	Fr
N	-	C	C	A		?	?	?	?	P	C
P		-	-	-		-	-	-		-	P
Cl	-	-	N	-	?	K	-	K	K	K	?
V	-	-	-	-		-	-	-	I	-	-
Cr	-	L	1	A		?	?	?	I	-	?
As		-	-			?	-	-	I		P
Br	?	?	N	K	?	K	-	K	K	K	?
Nb	12	L	234	3	-	-	124	-		-	-
Sb			-	I		I	I		N	-	
I	-	-	N	-	-	1		1	1	K	-
Ta	1	L	124	12	-	45	1234	P		-	P

A / B	H	Li	Na	K	Cu	Rb	Ag	Cs	Au	Tl	Fr
W	P	L	1	?	-		P	P			P
Re	P	L	?	?	-		P	P			P
Bi	I	-	I	-	-		P	P		P	1
At	?	?	?	?	?		P	P	P	1	1
Pa	P	L	2	1	P	1			P		1
U	P	L	2,3	1	P	1			P	1	P
Np	P	L	P	P							-
Pu	P	L	?	P	-		P	P		P	?

3.9.2.1.4. Analyse of Semantic Networks and Corresponding Logical Expressions

Table 3.9.2.1.4 contains the results of analyse for various classes and for description of elements A^{I} and B^{V} in terms of feature set IV.

Table 3.9.2.1.4
Result of Analyse of Pyramidal Network (Feature Set IV)
(Prediction of Crystal Structure Type)

Conjunction	Number of recurrences
Perovskite	
S, C9	17
I11, TM2	16
I11, TM2, E1	16
I11, E1	16
TM2, E1	16
S, R10	12
I11, H2	12
H2, I210	11
I11, TM2, E1, H2, I210	11
I11, TM2, H2, I210	11
S, C9, I11, TM2, H2, I210	11
S, I11, TM2, H2, I210	11
R10, TD1	11
E10, TM9	10
Calcite	
S, C9	2
I11, TM2	2
I210, H2	2
R1, I111	2
I11, H2	2
I11, H2, P	2
I11, TM2, I210, H2	2
S, C9, I11, TM2, H2, I210	2
S, C9, I11, TM2, H2, I210, TM1	2
S, I11, TM2, H2, I210	2
S, I11, TM2, H2, I210, I310	2
I39, S12	2
S, C9, I11, TM2, H2, I210, TM1, I39, S12	2
R1, I111, H1, I49	2
S, C9, I11, TM2, H2, I210, R1, I111, TM1, I39, S12, H1, I49	2
S, C9, I11, TM2, H2, I210, R1, I111, TM1, I310, I39, H1, I49, S12	2
I210, P	2
S, C9, I210, P	2
S, C9, I210, P, I39, S12	2

Conjunction	Number of recurrences
$LiNbO_3$	
I11, TM2	3
I210, H2	3
I11, H2	3
I11, TM2, I210, H2	3
I11, TM2, I210, H2, S	3
I11, TM2, I210, H2, S, I310	3
TD8, S2	3
C3, R4	3
TD8, S2, C3, R4	3
I11, TM2, I210, H2, S, I310, TD8, S2, C3, R4, E2	3
Ilmenite	
I33, I44	4
S, C9	3
I11, TM2	3
I11, TM2, E1	3
I11, E1	3
TM2, E1	3
S, R10	3
P, TM4	3
I33, I44, P, TM4	3
E4, TD6	3
E4, TD6, C4, R3, I18, I25, S6, H8	3
I33, I44, P, TM4, E4, TD6, C4, R3, I18, I25, S6, H8	3
$KBrO_3$	
R10, TD1	8
P, C10	8
P, C10, TM1	7
I29, I111	7
P, C10, TM1, I29, I111	7
R10, TD1, I39	5
R10, TD1, I29, I111, I39	5
R10, S	5
I11, E1	5

Conjunction	Number of recurrences
$NaClO_3$	
S, C9	3
I11, TM2	3
I11, TM2, E1	3
I210, H2	3
I11, TM2, E1, I210, H2	3
I11, TM2, E1, I210, H2, S7	3
I11, TM2, E1, I210, H2, S7, R8, I310, I410, TD4	3
I11, H2	3
I11, H2, P	3
I11, TM2, I210, H2	3
P, C10	3
I11, TM2, E1, I210, H2, S7, R8, I310, I410, TD4, P	3
S, C9, I11, TM2, I210, H2	3
S, I11, TM2, I210, H2	3
S, I11, TM2, I210, H2, I310	3
S, I11, TM2, E1, I210, H2, S7, R8, I310, I410, TD4,P	3
S, I11, TM2, E1, I210, H2, S7, R8, I310, I410, TD4, P, C10	3
I210, P	3
I11, E1	3
TM2, E1	3
S, C9, I210, P	3

Analyse of Table 3.9.2.1.4 shows that the perovskites with composition $A^{I}B^{V}O_3$ contain at least one element having heat of melting in the range from 2.2 to 4.6 kJ/mol and the second ionization potential in the range from 27.56 to 75.62 eV, or ionic radius in the range from 1.11 to 2.2 A and Debye temperature in the range from 39.2 to 90 K, or energy of the crystal lattice in the range from $652*10^{-6}$ to $905*10^{-6}$ J/kg**mol and melting point in the range from 2473 to 3660 K. The calcites of this composition contain at least one element having ionic radius by 0.39 A and first ionization potential in the range from 10.55 to 25 eV, or third ionization potential in the range from 37 to 47.426 eV and entropy of individual substances at 298 K in the range between 152 and 224 kJ/kg*mol*K, and so forth. The considerabl intersections of fields of classes in multidimensional space of feature set IV are obtained.

Table 3.9.2.1.5 contains the results of analyse for various classes and for description of compounds in terms of feature set VIII.

Table 3.9.2.1.5
Result of Analyse of Pyramidal Network (Feature Set VIII)
(Prediction of Crystal Structure Type)

Conjunction	Number of recurrences
Perovskite	
V1, V5, H13	17
R12, TM3	11
V1, V5, R12, TM3	11
Calcite	
R1, TM1	2
V1, V5, C10	2
V1, V5, R1, TM1, C10, H1	2
$LiNbO_3$	
V1, V5, H13	3
H7, C4, R5, TM5	3
V1, V5, H13, H7, C4, R5, TM5	3
V1, V5, H7, C4, R5, TM5	3
Ilmenite	
H9, C9	3
H9, C9, R3, TM2	3

Analyse of Table 3.9.2.1.5 shows that the fields of structure types of compounds with composition $A^{I}B^{V}O_3$ don't intersect in the multidimensional space of feature set of simple oxides. Thus this feature set is better for prediction of structure type than previous one.

Tables 3.9.2.1.6 and 3.9.2.1.7 contain the results of analyse of pyramidal networks for prediction of various types of distortion of ideal perovskite cell and for various description of elements A and B in terms of feature sets IV and VIII.

Table 3.9.2.1.6
Result of Analyse of Pyramidal Network (Feature Set IV)

Conjunction	Number of recurrences
Cubic Perovskite	
S, C9	11
I11, TM2	10
I11, TM2, E1	10
I11, E1	10
TM2, E1	10

Conjunction	Number of recurrences
Monoclinic Perovskite	
S, R4	5
S, R4, D	5
E10, TM9	5
E10, TM9, TD7	5
S, R4, D, E10, TM9, TD7	5
R4, E10, TM9, TD7	5
Rhombic Perovskite	
S, C9	6
D, R4	6
E10, TM9	6
D, R4, E10, TM9, TD7	6
I11, TM2	5
I11, TM2, I210, H2	5
I11, TM2, I210, H2, E1	5
S, I11, TM2, I210, H2	5
TM2, E1	5
I11, TM2, E1	5
S, C9, I11, TM2, E1	5

Table 3.9.2.1.7
Result of Analyse of Pyramidal Network (Feature Set VIII)

Conjunction	Number of recurrences
Cubic Perovskite	
V1, V5, H13	11
V1, V5, TM3	8
V1, V5, R12, TM3	8
V1, V5, H13, C10, R4	6
V1, V5, H13, TM6	6
V1, V5, TM3, R12, C7	6
V1, V5, H13, C10, R4, C6	5
V1, V5, H13, TM5	5
Monoclinic Perovskite	
V1, V5, C10	5
V1, V5, C10, H13, R4	5
V1, V5, H13	5
V1, V5, C10, H13, R4, C6	4
V1, V5, C10, H13, R4, TM6	3
C6, TM4	3

Conjunction	Number of recurrences
Rhombic Perovskite	
V1, V5, C6	7
V1, V5, C6, TM4	6
H13, C10, R4	5
V1, V5, H13, C10, R4	5
Hexagonal Perovskite	
V1, V5, H13	4
V1, V5, H13, TM5	3
C6, TM4	3
C10, R4	3
V1, V5, H13, C10, R4	3

Analyse of these Tables shows that the fields of various structure types of compounds with composition $A^{I}B^{V}O_3$ intersect very much in the multidimensional space of both feature sets: IV and VIII.

3.9.2.2. Predicting Crystal Structure Type of New Compounds with Composition $A^{II}B^{IV}O_3$

3.9.2.2.1. Data for Computer Learning

The data for computer learning was extracted from the DB on ternary inorganic compound properties [18-21]. Table 3.9.2.2.1 contains a resulting learning set.

Table 3.9.2.2.1
Learning Set for Predicting Possibility of Formation and Crystal Structure Types of Compounds with Compositionn $A^{II}B^{IV}O_3$

Composition	Crystal type	Space group or symmetry
MgSeO3	perovskite	rhombic
MgTeO3	perovskite	rhombic
MgCeO3	perovskite	cubic, monoclinic
MgThO3	perovskite	cubic
CaTiO3	perovskite	rhombic (GdFeO3)
CaVO3	perovskite	rhombic, cubic
CaCrO3	perovskite	rhombic (GdFeO3)
CaMnO3	perovskite	rhombic, cubic, monoclinic
CaZrO3	perovskite	rhombic (GdFeO3), monoclinic
CaNbO3	perovskite	rhombic (GdFeO3), monoclinic
CaMoO3	perovskite	rhombic (GdFeO3)
CaTcO3	perovskite	rhombic (GdFeO3)
CaRuO3	perovskite	rhombic, cubic

Composition	Crystal type	Space group or symmetry
CaHfO3	perovskite	monoclinic
CaIrO3	perovskite	rhombic
CaOsO3	perovskite	rhombic (GdFeO3)
CaUO3	perovskite	rhombic
CaThO3	perovskite	cubic, monoclinic
CaUO3	perovskite	cubic, rhombic
SrTiO3	perovskite	cubic
BaTiO3	perovskite	cubic, tetragonal
EuTiO3	perovskite	cubic
SrVO3	perovskite	cubic
CdVO3	perovskite	rhombic (GdFeO3)
BaVO3	perovskite	hexagonal
EuVO3	perovskite	monoclinic
SrCrO3	perovskite	cubic
PbCrO3	perovskite	cubic
MnSeO3	perovskite	rhombic
SrMnO3	perovskite	hexagonal
MnTeO3	perovskite	rhombic (GdFeO3)
BaMnO3	perovskite	hexagonal
PbMnO3	perovskite	?
MnPuO3	perovskite	rhombic (GdFeO3)
BaFeO3	perovskite	hexagonal, tetragonal
CoSeO3	perovskite	rhombic
CoTeO3	perovskite	rhombic
BaCoO3	perovskite	hexagonal
NiSeO3	perovskite	rhombic
BaNiO3	perovskite	hexagonal
CuTeO3	perovskite	rhombic
CuLaO3	perovskite	hexagonal
ZnSeO3	perovskite	rhombic
SrZrO3	perovskite	rhombic
SrNbO3	perovskite	hexagonal
SrMoO3	perovskite	cubic
SrTcO3	perovskite	cubic
SrRuO3	perovskite	rhombic (GdFeO3)
		cubic, monoclinic
SrSnO3	perovskite	cubic, monoclinic, rhombic
SrCeO3	perovskite	monoclinic, tetragonal
SrPrO3	perovskite	rhombic (GdFeO3)
SrTbO3	perovskite	rhombic (GdFeO3)
SrHfO3	perovskite	rhombic (GdFeO3)
		cubic, monoclinic
SrOsO3	perovskite	rhombic (GdFeO3)
SrIrO3	perovskite	monoclinic
SrPbO3	perovskite	rhombic (GdFeO3), monoclinic
SrThO3	perovskite	cubic, monoclinic
SrPaO3	perovskite	?
SrUO3	perovskite	rhombic (GdFeO3), hexagonal

Composition	Crystal type	Space group or symmetry
SrNpO3	perovskite	?
SrPuO3	perovskite	cubic, monoclinic, rhombic, hexagonal
SrAmO3	perovskite	cubic
CdZrO3	perovskite	monoclinic
BaZrO3	perovskite	cubic
EuZrO3	perovskite	cubic
PbZrO3	perovskite	rhombic
BaNbO3	perovskite	cubic
EuNbO3	perovskite	cubic
BaMoO3	perovskite	cubic
BaTcO3	perovskite	cubic, hexagonal
BaRuO3	perovskite	hexagonal
LaRuO3	perovskite	rhombic (GdFeO3), cubic
PbRuO3	perovskite	rhombic (GdFeO3), cubic
CdCeO3	perovskite	cubic, monoclinic
CdHfO3	perovskite	rhombic
CdOsO3	perovskite	rhombic
CdThO3	perovskite	cubic, monoclinic
BaSnO3	perovskite	cubic
SnTaO3	perovskite	?
BaCeO3	perovskite	cubic, rhombic monoclinic, tetragonal
BaPrO3	perovskite	cubic, rhombic, monoclinic
BaTbO3	perovskite	rhombic, hexagonal
BaHfO3	perovskite	cubic
BaOsO3	perovskite	hexagonal
BaIrO3	perovskite	hexagonal, monoclinic
BaPtO3	perovskite	hexagonal
BaPbO3	perovskite	cubic, monoclinic
BaThO3	perovskite	cubic, rhombic
BaPaO3	perovskite	cubic
BaUO3	perovskite	cubic
BaNpO3	perovskite	cubic
BaPuO3	perovskite	cubic
BaAmO3	perovskite	cubic
BaCmO3	perovskite	cubic
BaCfO3	perovskite	?
PbCeO3	perovskite	cubic, monoclinic
RaCeO3	perovskite	cubic
EuHfO3	perovskite	cubic
EuUO3	perovskite	rhombic
EuNpO3	perovskite	rhombic (GdFeO3)
HgTiO3	LiNbO3	R3c
MgCO3	calcite	R3(-)c
CaCO3	calcite	R3(-)c
MnCO3	calcite	R3(-)c
FeCO3	calcite	R3(-)c
CoCO3	calcite	R3(-)c

Composition	Crystal type	Space group or symmetry
NiCO3	calcite	R3(-)c
CuCO3	calcite	R3(-)c
ZnCO3	calcite	R3(-)c
CdCO3	calcite	R3(-)c
SrCO3	aragonite	Pmcn, Z=4
BaCO3	aragonite	Pmcn, Z=4
SmCO3	aragonite	Pmcn, Z=4
EuCO3	aragonite	Pmcn, Z=4
YbCO3	aragonite	Pmcn, Z=4
PbCO3	aragonite	Pmcn, Z=4
RaCO3	aragonite	Pmcn, Z=4
MgTiO3	ilmenite	R3(-)
MgNbO3	ilmenite	R3(-)
MgSnO3	ilmenite	R3(-)
CaSnO3	ilmenite	R3(-)
CaPbO3	ilmenite	R3(-)
MnTiO3	ilmenite	R3(-)
FeTiO3	ilmenite	R3(-)
CoTiO3	ilmenite	R3(-)
NiTiO3	ilmenite	R3(-)
ZnTiO3	ilmenite	R3(-)
CdTiO3	ilmenite	R3(-)
MnVO3	ilmenite	R3(-)
CoMnO3	ilmenite	R3(-)
NiMnO3	ilmenite	R3(-)
MnSnO3	ilmenite	R3(-)
FeNbO3	ilmenite	R3(-)
CdPbO3	ilmenite	R3(-)
MgSiO3	clinoenstatite	P2(1)/c, Z=8
MgVO3		Cmc2(1), Cmmm
MgGeO3	enstatite	Pbca, Z=16
MgMoO3		hexagonal
CaSiO3	wollastonite	P1(-), Z=12 (24)
MnSiO3		P1(-), Z=10
FeSiO3	orthopyroxene	Pbca, Z=16
CoSiO3	orthopyroxene	Pbca, Z=16
NiSiO3		rhombic
SrSiO3		C2, Z=12
CdSiO3		rhombic
BaSiO3		P2(1)2(1)2(1) (P222), Z=4
SmSiO3	pseudowollastonite	hexagonal
EuSiO3		C2
PbSiO3		P2/n, Z=12
MnSO3	alpha-FeSO3	R3(-)
FeSO3	alpha-FeSO3	R3(-)
CdSO3		P2(1)/c, Z=4
PbSO3		P2(1)/m, Z=2; Pnma, Z=4
CaGeO3	wollastonite	P1(-)
PdTiO3		rhombic

Composition	Crystal type	Space group or symmetry
CuVO3		R3(-)
BaCrO3		P6(3)/mmc, Z=14
ZnMnO3		cubic
MnGeO3	enstatite	Pbca, Z=16
SrFeO3		cubic
FeMoO3		hexagonal
CoGeO3	clinopyroxene	C2/c, Z=8
CoSnO3	rutile	P4/mnm
CoUO3		cubic
NiTeO3		Pnma, Z=4; C2/c
CuGeO3		rhombic
CuSeO3		Pcab, Z=8
CuNbO3		C2/m, Z=8
CuTaO3		R3c
ZnTeO3		Pbca, Z=8
SrGeO3	wollastonite	P1(-)
CdGeO3	pyroxene	Pmab, Z=4
BaGeO3	wollastonite	P1(-)
PbGeO3		P2/n, Z=12
CdSeO3		Pnma, Z=4
PbSeO3		P2(1)/m, Z=2
SrTeO3		triclinic
PbRhO3	pyrochlore	
CdSnO3	spinel	
CdTeO3		P2(1)/c, Z=8
CdUO3		cubic, Z=16
PbSnO3	pyrochlore	
BaTeO3	KClO3	P2(1)/m, Z=2
HgTeO3		P1(-), Z=4
PbTeO3		Amam, Z=24
PbHfO3		rhombic
PbOsO3	pyrochlore	
PbIrO3	pyrochlore	
BeCO3		
BeSO3		
BeSnO3		
TiCO3		
HgCO3		
MgSO3		
MgPbO3		
CuSiO3		
ZnSiO3		
SnSiO3		
YbSiO3		
CaSO3		
CrSO3		
CoSO3		
CuSO3		

Composition	Crystal type	Space group or symmetry
SrSO3		
SnSO3		
BaSO3		
OsSO3		
HgSO3		
CaSeO3		
CaTeO3		
CuTiO3		
CoVO3		
NiVO3		
FeMnO3		
CdMnO3		
PbFeO3		
NiMoO3		
CuPbO3		
ZnZrO3		
ZnSnO3		
SrSeO3		
BaSeO3		
HgSeO3		
SrPdO3		
SrPdO3		
LaNbO3		
BaPdO3		
LaPdO3		
SnHfO3		
BaReO3		
BaPoO3		
BaBkO3		
PbUO3		

Pseudo-Binary Systems in which Compound of Composition ABO_3 does not Form

BeO-ZrO2	without compound ABO3
BeO-RuO2	without compound ABO3
BeO-CeO2	without compound ABO3
BeO-ThO2	without compound ABO3
BeO-UO2	without compound ABO3
BeO-PuO2	without compound ABO3
MgO-RuO2	without compound ABO3
MgO-HfO2	without compound ABO3
MgO-UO2	without compound ABO3
MgO-PuO2	without compound ABO3
V-Si-O	without compound ABO3
Ti-W-O	without compound ABO3
FeO-ZrO2	without compound ABO3
NiO-HfO2	without compound ABO3
PdO-RuO2	without compound ABO3
PbO-PuO2	without compound ABO3

At first we predicted the possibility of forming compounds of composition $A^{II}B^{IV}O_3$ (divided into two classes - dichotomy). Next, we predicted the above-mentioned for $A^{I}B^{V}O_3$ crystal types at standard conditions (at room temperature and normal pressure) for predicted on the first stage compounds (multiclass predicting).

3.9.2.2.2. Selection of Features

On the basis of physical-chemical grounds three sets of constituent component features were selected for the description of oxide systems and compounds.

The first feature set coincides with Set V (see Section 3.6.2).

The second feature set coincides with Set IV (see Section 3.5.1.2.2).

The third feature set coincides with Set VIII (see Section 3.9.2.1.2).

3.9.2.2.3. Prediction of Formation

In the case of predicting the formation of the compounds with composition $A^{II}B^{IV}O_3$ the computer learning is carried out for three learning sets in which the compounds from Table 3.9.2.2.1 were described in terms of the sets of the component properties VI, V, and VIII. The system of concept formation CONFOR [14] was used for computer learning and prediction.

In the case of the descriptions in terms of feature sets IV and V, some of the objects from Table 3.9.2.2.1 were selected for the examination. The results of examination for feature sets IV and V testify (Tables 3.9.2.2.2 and 3.9.2.2.4) that errors of recognition in the case of the description in terms of the distribution of electrons in the shells of separate atoms, the ionic radii, and the corresponding formal valence (Feature set V) and in the case of the description in terms of the type of incomplete electronic shell, electronegative, first, second, third, and fourth ionization potentials, standard entropies, Debye temperature, melting point, heat of melting, ionic radius, standard capacity, and formal valency of elements A and B are practically equally (Tables 3.9.2.2.3 and 3.9.2.2.5). From the result obtained it may be deduced that these feature sets are practically equally important for prediction of formation of compounds with composition $A^{II}B^{IV}O_3$.

Table 3.9.2.2.2
Set for Examination (Feature Set V)

Composition	Class	Result of examination
BeCO3	compound ABO3 exists	X
BeSnO3	compound ABO3 exists	X
CaCO3	compound ABO3 exists	X
MnCO3	compound ABO3 exists	compound ABO3 exists
CoCO3	compound ABO3 exists	compound ABO3 exists
EuCO3	compound ABO3 exists	X
HgCO3	compound ABO3 exists	compound ABO3 exists
RaCO3	compound ABO3 exists	compound ABO3 exists
MgSO3	compound ABO3 exists	compound ABO3 exists
MgVO3	compound ABO3 exists	compound ABO3 exists
MgMnO3	compound ABO3 exists	compound ABO3 exists
MgCoO3	compound ABO3 exists	compound ABO3 exists
MgSeO3	compound ABO3 exists	compound ABO3 exists
MgNbO3	compound ABO3 exists	X
MgTeO3	compound ABO3 exists	compound ABO3 exists
MnSiO3	compound ABO3 exists	compound ABO3 exists
CdSiO3	compound ABO3 exists	compound ABO3 exists
SmSiO3	compound ABO3 exists	X
PbSiO3	compound ABO3 exists	compound ABO3 exists
CrSO3	compound ABO3 exists	compound ABO3 exists
CdSO3	compound ABO3 exists	compound ABO3 exists
OsSO3	compound ABO3 exists	X
CaVO3	compound ABO3 exists	compound ABO3 exists
CaZrO3	compound ABO3 exists	compound ABO3 exists
CaMoO3	compound ABO3 exists	compound ABO3 does not form
CaRuO3	compound ABO3 exists	compound ABO3 does not form
CaSnO3	compound ABO3 exists	compound ABO3 exists
CaOsO3	compound ABO3 exists	X
CaPbO3	compound ABO3 exists	X
CaUO3	compound ABO3 exists	X
MnTiO3	compound ABO3 exists	compound ABO3 exists
CoTiO3	compound ABO3 exists	compound ABO3 exists
NiTiO3	compound ABO3 exists	compound ABO3 exists
CuTiO3	compound ABO3 exists	compound ABO3 exists
ZnTiO3	compound ABO3 exists	compound ABO3 exists
EuTiO3	compound ABO3 exists	X
VMnO3	compound ABO3 exists	compound ABO3 exists
CuVO3	compound ABO3 exists	compound ABO3 exists
BaVO3	compound ABO3 exists	X
EuVO3	compound ABO3 exists	X
FeMnO3	compound ABO3 exists	compound ABO3 exists
MnGeO3	compound ABO3 exists	compound ABO3 exists
CdMnO3	compound ABO3 exists	compound ABO3 exists
PbMnO3	compound ABO3 exists	compound ABO3 exists
BaFeO3	compound ABO3 exists	X
PbFeO3	compound ABO3 exists	X
CoSnO3	compound ABO3 exists	compound ABO3 exists

Composition	Class	Result of examination
CoTeO3	compound ABO3 exists	compound ABO3 exists
BaNiO3	compound ABO3 exists	X
CuGeO3	compound ABO3 exists	compound ABO3 exists
CuSeO3	compound ABO3 exists	compound ABO3 exists
CuNbO3	compound ABO3 exists	compound ABO3 does not form
CuTeO3	compound ABO3 exists	compound ABO3 exists
CuTaO3	compound ABO3 exists	X
ZnGeO3	compound ABO3 exists	compound ABO3 exists
SrGeO3	compound ABO3 exists	compound ABO3 exists
BaGeO3	compound ABO3 exists	compound ABO3 exists
PbGeO3	compound ABO3 exists	compound ABO3 exists
CdSeO3	compound ABO3 exists	compound ABO3 exists
SrTcO3	compound ABO3 exists	compound ABO3 exists
SrPrO3	compound ABO3 exists	compound ABO3 exists
SrTbO3	compound ABO3 exists	compound ABO3 exists
SrOsO3	compound ABO3 exists	compound ABO3 exists
SrIrO3	compound ABO3 exists	compound ABO3 exists
SrPaO3	compound ABO3 exists	compound ABO3 exists
SrPuO3	compound ABO3 exists	compound ABO3 exists
SrAmO3	compound ABO3 exists	compound ABO3 exists
CdZrO3	compound ABO3 exists	compound ABO3 does not form
BaMoO3	compound ABO3 exists	compound ABO3 exists
BaRuO3	compound ABO3 exists	compound ABO3 exists
PbRhO3	compound ABO3 exists	compound ABO3 exists
LaPdO3	compound ABO3 exists	compound ABO3 exists
CdSnO3	compound ABO3 exists	compound ABO3 does not form
CdTeO3	compound ABO3 exists	compound ABO3 does not form
CdUO3	compound ABO3 exists	compound ABO3 exists
BaSnO3	compound ABO3 exists	compound ABO3 exists
SnHfO3	compound ABO3 exists	compound ABO3 exists
SnTaO3	compound ABO3 exists	compound ABO3 exists
BaPrO3	compound ABO3 exists	compound ABO3 exists
BaIrO3	compound ABO3 exists	compound ABO3 exists
BaPoO3	compound ABO3 exists	compound ABO3 exists
BaUO3	compound ABO3 exists	compound ABO3 exists
BaCmO3	compound ABO3 exists	compound ABO3 exists
PbCeO3	compound ABO3 exists	compound ABO3 exists
RaCeO3	compound ABO3 exists	compound ABO3 exists
EuNpO3	compound ABO3 exists	compound ABO3 exists
PbOsO3	compound ABO3 exists	compound ABO3 exists
PbUO3	compound ABO3 exists	compound ABO3 does not form
SrCO3	compound ABO3 exists	compound ABO3 exists
CoSiO3	compound ABO3 exists	compound ABO3 exists
SrZrO3	compound ABO3 exists	compound ABO3 exists
BaNbO3	compound ABO3 exists	compound ABO3 exists
BeO-ThO2	compound ABO3 does not form	X
BeO-UO2	compound ABO3 does not form	X
BeO-PuO2	compound ABO3 does not form	X
MgO-HfO2	compound ABO3 does not form	X

Composition	Class	Result of examination
MgO-UO2	compound ABO3 does not form	X
MgO-PuO2	compound ABO3 does not form	X
Ti-W-O	compound ABO3 does not form	X
PdO-RuO2	compound ABO3 does not form	compound ABO3 does not form

Table 3.9.2.2.3
ESTIMATION OF RESULTS OF EXAMINATION (Feature Set V)

Class of compound ABO3 :
number of objects - 92 ;
correctly - 68 [73.913043 %] ;
incorrectly - 7 [7.6086957 %] ;
indeterminately - 17 [18.478261 %] ;

Class without compound ABO3 :
number of objects - 8 ;
correctly - 1 [12.5 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 7 [87.5 %] ;

Number of objects - 100 ;
correctly - 69 [69 %] ;
incorrectly - 7 [7 %] ;
indeterminately - 24 [24 %] ;

Table 3.9.2.2.4
Set for Examination (Feature Set IV)

Composition	Class	Result of examination
PbHfO3	compound ABO3 exists	X
BaPbO3	compound ABO3 exists	X
BaPdO3	compound ABO3 exists	X
SrPbO3	compound ABO3 exists	X
PbSeO3	compound ABO3 exists	compound ABO3 does not form
ZnZrO3	compound ABO3 exists	compound ABO3 exists
PbCrO3	compound ABO3 exists	X
CdVO3	compound ABO3 exists	compound ABO3 exists
PbTiO3	compound ABO3 exists	X
PdTiO3	compound ABO3 exists	X
CaTcO3	compound ABO3 exists	X
CaCeO3	compound ABO3 exists	compound ABO3 exists
CaHfO3	compound ABO3 exists	compound ABO3 exists
CaThO3	compound ABO3 exists	compound ABO3 exists
PbSO3	compound ABO3 exists	compound ABO3 does not form
CaTiO3	compound ABO3 exists	compound ABO3 exists
MgSnO3	compound ABO3 exists	compound ABO3 exists

Composition	Class	Result of examination
MgCeO3	compound ABO3 exists	compound ABO3 does not form
MgGeO3	compound ABO3 exists	X
BeSO3	compound ABO3 exists	X
MgCO3	compound ABO3 exists	X
TiCO3	compound ABO3 exists	compound ABO3 exists
NiCO3	compound ABO3 exists	compound ABO3 exists
ZnCO3	compound ABO3 exists	compound ABO3 exists
BaCO3	compound ABO3 exists	compound ABO3 exists
SmCO3	compound ABO3 exists	compound ABO3 exists
PbCO3	compound ABO3 exists	compound ABO3 does not form
MgSiO3	compound ABO3 exists	X
MgTiO3	compound ABO3 exists	compound ABO3 exists
MgMoO3	compound ABO3 exists	compound ABO3 exists
MgThO3	compound ABO3 exists	compound ABO3 exists
CaSiO3	compound ABO3 exists	compound ABO3 exists
FeSiO3	compound ABO3 exists	compound ABO3 exists
NiSiO3	compound ABO3 exists	compound ABO3 exists
SrSiO3	compound ABO3 exists	compound ABO3 exists
SnSiO3	compound ABO3 exists	compound ABO3 exists
EuSiO3	compound ABO3 exists	compound ABO3 exists
YbSiO3	compound ABO3 exists	compound ABO3 exists
MnSO3	compound ABO3 exists	compound ABO3 exists
CoSO3	compound ABO3 exists	compound ABO3 exists
SrSO3	compound ABO3 exists	compound ABO3 exists
BaSO3	compound ABO3 exists	compound ABO3 exists
CaSeO3	compound ABO3 exists	compound ABO3 exists
FeTiO3	compound ABO3 exists	compound ABO3 exists
SrTiO3	compound ABO3 exists	compound ABO3 exists
MnTeO3	compound ABO3 exists	compound ABO3 exists
BaTiO3	compound ABO3 exists	compound ABO3 exists
HgTiO3	compound ABO3 exists	compound ABO3 exists
CoVO3	compound ABO3 exists	compound ABO3 exists
NiVO3	compound ABO3 exists	X
CrMnO3	compound ABO3 exists	compound ABO3 exists
CoMnO3	compound ABO3 exists	compound ABO3 exists
SrMnO3	compound ABO3 exists	X
MnSnO3	compound ABO3 exists	compound ABO3 exists
BaMnO3	compound ABO3 exists	X
SrFeO3	compound ABO3 exists	compound ABO3 exists
FeNbO3	compound ABO3 exists	X
CoGeO3	compound ABO3 exists	compound ABO3 exists
SrCoO3	compound ABO3 exists	compound ABO3 exists
CoSeO3	compound ABO3 exists	compound ABO3 exists
BaCoO3	compound ABO3 exists	compound ABO3 exists
SrNiO3	compound ABO3 exists	compound ABO3 exists
NiTeO3	compound ABO3 exists	compound ABO3 exists
CuLaO3	compound ABO3 exists	X
CuPbO3	compound ABO3 exists	X
ZnTeO3	compound ABO3 exists	compound ABO3 exists

Composition	Class	Result of examination
CdGeO3	compound ABO3 exists	compound ABO3 exists
SrSeO3	compound ABO3 exists	compound ABO3 exists
BaSeO3	compound ABO3 exists	compound ABO3 exists
SrMoO3	compound ABO3 exists	compound ABO3 exists
SrRuO3	compound ABO3 exists	compound ABO3 exists
SrTeO3	compound ABO3 exists	compound ABO3 exists
SrCeO3	compound ABO3 exists	compound ABO3 exists
SrHfO3	compound ABO3 exists	compound ABO3 exists
SrThO3	compound ABO3 exists	compound ABO3 exists
SrNpO3	compound ABO3 exists	compound ABO3 exists
EuZrO3	compound ABO3 exists	compound ABO3 exists
LaNbO3	compound ABO3 exists	X
EuNbO3	compound ABO3 exists	X
BaRuO3	compound ABO3 exists	compound ABO3 exists
BaRhO3	compound ABO3 exists	compound ABO3 exists
CdCeO3	compound ABO3 exists	compound ABO3 exists
CdOsO3	compound ABO3 exists	compound ABO3 exists
CdThO3	compound ABO3 exists	compound ABO3 exists
BaTbO3	compound ABO3 exists	compound ABO3 exists
BaReO3	compound ABO3 exists	compound ABO3 exists
BaPuO3	compound ABO3 exists	compound ABO3 exists
BaCfO3	compound ABO3 exists	compound ABO3 exists
EuUO3	compound ABO3 exists	X
EuHfO3	compound ABO3 exists	compound ABO3 exists
HgTeO3	compound ABO3 exists	compound ABO3 exists
SrPdO3	compound ABO3 exists	X
CoUO3	compound ABO3 exists	compound ABO3 exists
SrCrO3	compound ABO3 exists	compound ABO3 exists
CaMnO3	compound ABO3 exists	X
ZnSiO3	compound ABO3 exists	compound ABO3 exists

Table 3.9.2.2.5
ESTIMATION OF RESULTS OF EXAMINATION (Feature Set IV)

Class of compound ABO3 :
number of objects - 96 ;
correctly - 69 [71.875 %] ;
incorrectly - 4 [4.1666667 %] ;
indeterminately - 23 [23.958333 %] ;

Number of objects - 96 ;
correctly - 69 [71.875 %] ;
incorrectly - 4 [4.1666667 %] ;
indeterminately - 23 [23.958333 %] ;

3.9.2.2.4. Analyse of Semantic Networks and Corresponding Logical Expressions

Table 3.9.2.2.6 contains the results of analyse for various classes and for description of elements A^{II} and B^{IV} in terms of feature set IV.

Table 3.9.2.2.6
Result of Analyse of Pyramidal Network (Feature Set IV)

Conjunction	Number of recurrences
Class of compounds with composition ABO_3	
S, E2	56
R10, TD2	56
S, E2, TM4	50
I12, I21	48
I16, I24	48
TD2, S8	46
TM4, I21	45
R10, TD2, TM4	44
S8, C7	44
TD2, S8, C7	44
TD2, S8, C7, H3	44
P, I36	43
P, E3	43
R10, TD2, TM4, I12, I21	42
S, E2, R10, TD2, TM4, I12, I21	42
I16, I24, H3	35
H3, TM3	35
D, TD9	33
I16, I24, I36	33
I47, H6	30
I16, I24, H3, P, I36	30
P, C2	28
I12, I21, I46	28
E3, I42	28
I310, I49	27
I310, H4	27
I16, I24, E4	27
I46, I38	27
H3, I25	26
S, E2, R10, TD2, TM4, I12, I21, I46, I38	26
S, E2, R10, TD2, TM4, I12, I21, S8, C7, H3, I46, I38	26
I24, S3	26
S7, TD5	25
TD2, S8, I42	25

Conjunction	Number of recurrences
Without compound ABO_3	
I310, TD11	7
S, TM6	7
R1, S1	7
TM6, C1	6
TM6, C1, I110	6
I26, I410	6
E5, H5	6
I310, TD11, C1	6
TM6, C1, I110, I26, I410	6
S, TM6, E5, H5	6
I310, TD11, S, TM6, R1, S1, C1, I110, I26, I410, E5, H5	6

Analyse of Table 3.9.2.2.6 shows that the compounds with composition $A^{II}B^{IV}O_3$ contain at least one s-element having energy of the crystal lattice in the range from $130*10^{-6}$ to $182.8*10^{-6}$ J/kg*mol, or ionic radius in the range from 1.11 to 2.2 A and Debye temperature in the range between 90 and 129 K, or the first ionization potential in the range from 5.39 to 5.9 eV and the second ionization potential less then 11.5 eV, and so forth. The good division of two classes is obtained in feature space IV.

Table 3.9.2.2.7 contains the results of analyse for various classes and for description of elements A^{II} and B^{IV} in terms of feature set VIII.

Table 3.9.2.2.7
Result of Analyse of Pyramidal Network (Feature Set VIII)

Conjunction	Number of recurrences
Class of compounds with composition ABO_3	
V2, V4, C2	91
V2, V4, TM6	89
V2, C3	85
V2, V4, C3	84
H7, TM8	76
V2, V4, R6	61
H7, TM8, R11	51
V2, V4, TM6, C3	46
V2, V4, H8	43
H3, TM4	42
TM6, H7	40

Conjunction	Number of recurrences
TM6, C4	37
V2, V4, C1	33
TM6, H7, R12	32
V2, TM6, C3, H7, R12	32
V2, V4, C2, TM6	32
V2, V4, TM6, C3, H7, R12	31
V2, V4, C3, H7, TM8, R11	30
V2, V4, TM6, R6	29
TM4, R2	29
V2, V4, H8, R2	28
TM4, H4	27
TM6, H3	27
V2, V4, TM6, H8	25
Without compound ABO_3	
V2, V4, C1	11
H7, TM8	10
V2, V4, R6	8
V2, V4, C1, R1	6
V2, V4, C1, H7, R1	6
V2, V4, C1, H7, TM8, R1	6

Analyse of Table 3.9.2.2.7 shows that the compounds with composition $A^{II}B^{IV}O_3$ are formed at least one oxide having standard capacity in the range from 9.036 to 10.54 cal/mol*K , or the melting point in the range from 2000 to 2270 K, or standard capacity in the range from 10.54 to 11.9 cal/mol*K, and so forth. The systems without compounds of this composition contain at least one simple oxide having standard capacity in the range from 6.09 to 9.036 cal/mol*K, or standard heat of formation in the range from 138.81 to 151.79 kcal/mol and the melting point in the range from 2660 to 3330 K, and so forth.

3.9.2.2.5. Prediction of Crystal Structure

In the case of predicting the crystal structure type of the compounds with composition $A^{II}B^{IV}O_3$ the computer learning is carried out for three learning sets in which the compounds from Table 3.9.2.2.1 were described in terms of the sets of the component properties VI, V, and VIII also. The system of concept formation CONFOR [14] was used for computer learning and prediction also.

In the case of the descriptions in terms of feature sets IV and V, some of the objects from Table 3.9.2.2.1 were selected for the examination also. The results of examination for feature sets IV and V testify (Tables 3.9.2.2.8 and 3.9.2.2.10) that there is a vagueness

of recognition which suggests that the level of the computer training is rather bad (Tables 3.9.2.2.9 and 3.9.2.2.11). But an error of recognition in the case of the description in terms of the distribution of electrons in the shells of separate atoms, the ionic radii, and the corresponding formal valence (Feature set V) is more than it is in the case of the description in terms of the type of incomplete electronic shell, electronegative, first, second, third, and fourth ionization potentials, standard entropies, Debye temperature, melting point, heat of melting, ionic radius, standard capacity, and formal valency (Feature set IV). From the result obtained it may be deduced that the feature set IV is better for prediction of crystal structure types of compounds with composition $A^{II}B^{IV}O_3$.

Table 3.9.2.2.8
Set for Examination (Feature Set V)

Composition	Class	Result of examination
MgThO3	perovskite	X
CaMnO3	perovskite	X
CaNbO3	perovskite	X
CaHfO3	perovskite	X
CaUO3	perovskite	X
MnTeO3	perovskite	X
SrVO3	perovskite	X
MnPuO3	perovskite	X
BaCoO3	perovskite	X
SrNiO3	perovskite	X
ZnSeO3	perovskite	X
SrTcO3	perovskite	perovskite
SrSnO3	perovskite	X
SrHfO3	perovskite	X
SrThO3	perovskite	X
SrUO3	perovskite	X
SrPuO3	perovskite	X
EuZrO3	perovskite	X
CdHfO3	perovskite	X
CdThO3	perovskite	X
BaPrO3	perovskite	perovskite
BaIrO3	perovskite	X
BaPaO3	perovskite	X
BaNpO3	perovskite	X
BaCfO3	perovskite	X
MnCO3	calcite	calcite
SrCO3	aragonite	X
BaCO3	aragonite	X
PbCO3	aragonite	X
MnTiO3	ilmenite	X
ZnTiO3	ilmenite	X
NiMnO3	ilmenite	X
CdPbO3	ilmenite	X

Composition	Class	Result of examination
FeSiO3	another structure	X
CdSO3	another structure	X
CdGeO3	another structure	X
SnPbO3	another structure	X
VVO3	another structure	X
MnMnO3	another structure	X
CoCoO3	another structure	X
BeO-UO2	without compound ABO3	X

Table 3.9.2.2.9
ESTIMATION OF RESULTS OF EXAMINATION (Feature Set V)

Class of perovskite :
number of objects - 25 ;
correctly - 2 [8 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 23 [92 %] ;

Class of calcite :
number of objects - 1 ;
correctly - 1 [100 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 0 [0 %] ;

Class of aragonite :
number of objects - 3 ;
correctly - 0 [0 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 3 [100 %] ;

Class of ilmenite :
number of objects - 4 ;
correctly - 0 [0 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 4 [100 %] ;

Class of another structure :
number of objects - 7 ;
correctly - 0 [0 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 7 [100 %] ;

Class without compound ABO3 :
number of objects - 1 ;
correctly - 0 [0 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 1 [100 %] ;

Number of objects - 41 ;
correctly - 3 [7.3170732 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 38 [92.682927 %] ;

Table 3.9.2.2.10
Set for Examination (Feature Set IV)

Composition	Class	Result of examination
SrVO3	perovskite	perovskite
SrNiO3	perovskite	perovskite
SrHfO3	perovskite	perovskite
SrUO3	perovskite	perovskite
BaHfO3	perovskite	X
BaNpO3	perovskite	X
BaNbO3	perovskite	X
BaPbO3	perovskite	X
CuTeO3	perovskite	X
MnSeO3	perovskite	X
CaVO3	perovskite	perovskite
CaTiO3	perovskite	perovskite
CaMoO3	perovskite	perovskite
CaThO3	perovskite	X
PbTiO3	perovskite	X
PbCrO3	perovskite	X
BaFeO3	perovskite	X
SrMoO3	perovskite	perovskite
SrTbO3	perovskite	perovskite
SrPaO3	perovskite	perovskite
BaZrO3	perovskite	X
BaTcO3	perovskite	X
CdOsO3	perovskite	perovskite
BaTbO3	perovskite	X
BaThO3	perovskite	X
BaCmO3	perovskite	X
MgCO3	calcite	X
BaCO3	aragonite	X
MgTiO3	ilmenite	X
FeTiO3	ilmenite	X
FeFeO3	another structure	another structure
BeO-RuO2	without compound ABO3	without compound ABO3

Table 3.9.2.2.11

ESTIMATION OF RESULTS OF EXAMINATION (Feature Set IV)

Class of perovskite :
- number of objects - 26 ;
- correctly - 11 [42.307692 %] ;
- incorrectly - 0 [0 %] ;
- indeterminately - 15 [57.692308 %] ;

Class of calcite :
- number of objects - 1 ;
- correctly - 0 [0 %] ;
- incorrectly - 0 [0 %] ;
- indeterminately - 1 [100 %] ;

Class of aragonite :
- number of objects - 1 ;
- correctly - 0 [0 %] ;
- incorrectly - 0 [0 %] ;
- indeterminately - 1 [100 %] ;

Class of ilmenite :
- number of objects - 2 ;
- correctly - 0 [0 %] ;
- incorrectly - 0 [0 %] ;
- indeterminately - 2 [100 %] ;

Class of another structure :
- number of objects - 1 ;
- correctly - 1 [100 %] ;
- incorrectly - 0 [0 %] ;
- indeterminately - 0 [0 %] ;

Class without compound ABO3 :
- number of objects - 1 ;
- correctly - 1 [100 %] ;
- incorrectly - 0 [0 %] ;
- indeterminately - 0 [0 %] ;

Number of objects - 32 ;
- correctly - 13 [40.625 %] ;
- incorrectly - 0 [0 %] ;
- indeterminately - 19 [59.375 %] ;

The pyramidal networks and the corresponding logical expressions were formed as a result of the computer learning via CONFOR. Appendix 10 contains the logical expressions for various learning sets.

In the case of predicting the distortion of ideal cubic cell of perovskite for the compounds with composition $A^{II}B^{IV}O_3$ the computer learning is carried out for each type of symmetry (cubic, monoclinic, rhombic, tetragonal, and hexagonal) and for three learning sets in which the compounds from Table 3.9.2.2.1 were described in terms of the sets of the component properties VI, V, and VIII.

In the case of the descriptions in terms of feature sets IV and V, some of the objects from Table 3.9.2.2.1 were selected for the examination also. The results of examination for feature set V were shown in:

Tables 3.9.2.2.12 and 3.9.2.2.13 - hexagonally distorted perovskite;
Tables 3.9.2.2.16 and 3.9.2.2.17 - ideal cubic perovskite;
Tables 3.9.2.2.20 and 3.9.2.2.21 - monoclinically distorted perovskite;
Tables 3.9.2.2.24 and 3.9.2.2.25 - rhombically distorted perovskite;
Tables 3.9.2.2.28 and 3.9.2.2.29 - tetragonally distorted perovskite;

The results of examination for feature set IV were shown in:

Tables 3.9.2.2.14 and 3.9.2.2.15 - hexagonally distorted perovskite;
Tables 3.9.2.2.18 and 3.9.2.2.19 - ideal cubic perovskite;
Tables 3.9.2.2.22 and 3.9.2.2.23 - monoclinically distorted perovskite;
Tables 3.9.2.2.26 and 3.9.2.2.27 - rhombically distorted perovskite;
Tables 3.9.2.2.30 and 3.9.2.2.31 - tetragonally distorted perovskite.

Table 3.9.2.2.12
Set for Examination (Feature Set V) / Hexagonally Distorted Perovskite

Composition	Class	Result of examination
CuLaO3	perovskite hex.	X
SrPuO3	perovskite hex.	X
BaPtO3	perovskite hex.	X
MnCO3	another structure	X
NiCO3	another structure	another structure
SrCO3	another structure	X
SmCO3	another structure	X
PbCO3	another structure	another structure
MgTiO3	another structure	another structure
MgSeO3	another structure	X
MgTeO3	another structure	X
CaSiO3	another structure	X
CoSiO3	another structure	another structure
CdSiO3	another structure	X
EuSiO3	another structure	X
FeSO3	another structure	another structure
CaTiO3	another structure	X
CaMnO3	another structure	X
CaRuO3	another structure	X
CaThO3	another structure	X
NiTiO3	another structure	another structure

Composition	Class	Result of examination
PdTiO3	another structure	X
EuTiO3	another structure	X
CdVO3	another structure	X
MnGeO3	another structure	another structure
CoSnO3	another structure	X
CuSeO3	another structure	another structure
PbGeO3	another structure	another structure
SrPrO3	another structure	X
SrThO3	another structure	X
BaZrO3	another structure	X
BaNbO3	another structure	X
LaRuO3	another structure	another structure
CdSnO3	another structure	X
CdHfO3	another structure	X
CdThO3	another structure	X
SnPbO3	another structure	X
HgTeO3	another structure	another structure
BaPrO3	another structure	X
BaThO3	another structure	X
BaNpO3	another structure	X
BaCmO3	another structure	X
RaCeO3	another structure	X
EuNpO3	another structure	X
PbIrO3	another structure	another structure
BeO-CeO2	without compound ABO3	X
MgO-UO2	without compound ABO3	X
Ti-W-O	without compound ABO3	X

Table 3.9.2.2.13
ESTIMATION OF RESULTS OF EXAMINATION (Feature Set V)
Hexagonally Distorted Perovskite

Class of perovskite hex. :
number of objects - 3 ;
correctly - 0 [0 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 3 [100 %] ;

Class of another structure :
number of objects - 42 ;
correctly - 12 [28.571429 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 30 [71.428571 %] ;

Class of without compound ABO3 :
number of objects - 3 ;
correctly - 0 [0 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 3 [100 %] ;

Number of objects - 48 ;
correctly - 12 [25 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 36 [75 %] ;

Table 3.9.2.2.14
Set for Examination (Feature Set IV)
Hexagonally Distorted Perovskite

Composition	Class	Result of examination
BaIrO3	perovskite hex.	X
FeCO3	another structure	another structure
ZnCO3	another structure	another structure
EuCO3	another structure	another structure
MgNbO3	another structure	another structure
MgThO3	another structure	another structure
NiSiO3	another structure	X
CdSO3	another structure	another structure
CaCrO3	another structure	another structure
CaMoO3	another structure	another structure
CaHfO3	another structure	X
CaPbO3	another structure	another structure
MnTiO3	another structure	another structure
ZnTiO3	another structure	another structure
EuVO3	another structure	X
PbCrO3	another structure	another structure
NiMnO3	another structure	X
MnSnO3	another structure	another structure
CoTeO3	another structure	another structure
CuTeO3	another structure	another structure
SrGeO3	another structure	another structure
CdSeO3	another structure	another structure
SrSnO3	another structure	another structure
SrAmO3	another structure	X
CdCeO3	another structure	another structure
CdUO3	another structure	another structure
BaUO3	another structure	another structure
LaLaO3	another structure	another structure
EuUO3	another structure	another structure
BeO-ThO2	without compound ABO3	X
BeO-PuO2	without compound ABO3	without compound ABO3

Table 3.9.2.2.15
ESTIMATION OF RESULTS OF EXAMINATION (Feature Set IV)
Hexagonally Distorted Perovskite

Class of perovskite hex. :
number of objects - 1 ;
correctly - 0 [0 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 1 [100 %] ;

Class of another structure :
number of objects - 28 ;
correctly - 23 [82.142857 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 5 [17.857143 %] ;

Class of without compound ABO3 :
number of objects - 2 ;
correctly - 1 [50 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 1 [50 %] ;

Number of objects - 31 ;
correctly - 24 [77.419355 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 7 [22.580645 %] ;

Table 3.9.2.2.16
Set for Examination (Feature Set V)
Ideal Cubic Perovskite

Composition	Class	Result of examination
MgCeO3	perovskite cub.	perovskite cub.
CaRuO3	perovskite cub.	X
EuTiO3	perovskite cub.	X
PbCrO3	perovskite cub.	X
SrSnO3	perovskite cub.	X
SrAmO3	perovskite cub.	X
EuZrO3	perovskite cub.	X
BaTcO3	perovskite cub.	X
BaSnO3	perovskite cub.	X
BaThO3	perovskite cub.	X
BaPuO3	perovskite cub.	X
RaCeO3	perovskite cub.	X
MnCO3	another structure	X
FeCO3	another structure	X
CoCO3	another structure	X
NiCO3	another structure	X
CuCO3	another structure	X
ZnCO3	another structure	another structure

Composition	Class	Result of examination
SmCO3	another structure	X
YbCO3	another structure	X
MnSiO3	another structure	X
FeSiO3	another structure	X
CoSiO3	another structure	X
NiSiO3	another structure	X
SmSiO3	another structure	X
MnSO3	another structure	X
FeSO3	another structure	X
MnGeO3	another structure	X
MnSeO3	another structure	X
MnTeO3	another structure	X
MnPuO3	another structure	X
FeFeO3	another structure	X
CoCoO3	another structure	X
CoGeO3	another structure	X
CoSeO3	another structure	X
CoTeO3	another structure	X
NiSeO3	another structure	X
NiTeO3	another structure	X
CuGeO3	another structure	X
CuSeO3	another structure	X
CuTeO3	another structure	X
CuLaO3	another structure	X
CuTaO3	another structure	X
ZnSeO3	another structure	X
ZnTeO3	another structure	X
SnPbO3	another structure	X
HgTeO3	another structure	another structure
LaLaO3	another structure	X
V-Si-O	without compound ABO3	X
Ti-W-O	without compound ABO3	X

Table 3.9.2.2.17
ESTIMATION OF RESULTS OF EXAMINATION (Feature Set V)
Ideal Cubic Perovskite

Class of perovskite cub. :
number of objects - 12 ;
correctly - 1 [8.3333333 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 11 [91.666667 %] ;

Class of another structure :
number of objects - 36 ;
correctly - 2 [5.5555556 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 34 [94.444444 %] ;

Class of without compound ABO3 :
number of objects - 2 ;
correctly - 0 [0 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 2 [100 %] ;

Number of objects - 50 ;
correctly - 3 [6 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 47 [94 %] ;

Table 3.9.2.2.18
Set for Examination (Feature Set IV)
Ideal Cubic Perovskite

Composition	Class	Result of examination
MgCeO3	perovskite cub.	X
EuTiO3	perovskite cub.	X
PbCrO3	perovskite cub.	another structure
EuZrO3	perovskite cub.	X
BaSnO3	perovskite cub.	X
BaPuO3	perovskite cub.	perovskite cub.
RaCeO3	perovskite cub.	another structure
MnCO3	another structure	another structure
CoCO3	another structure	another structure
NiCO3	another structure	X
CuCO3	another structure	another structure
ZnCO3	another structure	another structure
YbCO3	another structure	X
MnSiO3	another structure	another structure
FeSiO3	another structure	another structure
CoSiO3	another structure	another structure
NiSiO3	another structure	X
MnSO3	another structure	another structure
FeSO3	another structure	another structure
MnGeO3	another structure	another structure
MnSeO3	another structure	another structure
MnPuO3	another structure	another structure
FeFeO3	another structure	another structure
CoCoO3	another structure	another structure
CoGeO3	another structure	another structure
CoSeO3	another structure	another structure
CoTeO3	another structure	another structure
NiSeO3	another structure	X
NiTeO3	another structure	X
CuGeO3	another structure	another structure
CuSeO3	another structure	another structure
CuTeO3	another structure	another structure
CuLaO3	another structure	X
CuTaO3	another structure	another structure

Composition	Class	Result of examination
ZnSeO3	another structure	another structure
ZnTeO3	another structure	another structure
SnPbO3	another structure	another structure
HgTeO3	another structure	another structure
Ti-W-O	without compound ABO3	X

Table 3.9.2.2.19
ESTIMATION OF RESULTS OF EXAMINATION (Feature Set IV)
Ideal Cubic Perovskite

Class of perovskite cub. :
number of objects - 7 ;
correctly - 1 [14.285714 %] ;
incorrectly - 2 [28.571429 %] ;
indeterminately - 4 [57.142857 %] ;

Class of another structure :
number of objects - 31 ;
correctly - 25 [80.645161 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 6 [19.354839 %] ;

Class of without compound ABO3 :
number of objects - 1 ;
correctly - 0 [0 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 1 [100 %] ;

Number of objects - 39 ;
correctly - 26 [66.666667 %] ;
incorrectly - 2 [5.1282051 %] ;
indeterminately - 11 [28.205128 %] ;

Table 3.9.2.2.20
Set for Examination (Feature Set V)
Monoclinically Distorted Perovskite

Composition	Class	Result of examination
MnCO3	another structure	another structure
FeCO3	another structure	another structure
CoCO3	another structure	another structure
NiCO3	another structure	another structure
CuCO3	another structure	another structure
ZnCO3	another structure	X
SmCO3	another structure	X

Composition	Class	Result of examination
YbCO3	another structure	X
RaCO3	another structure	X
MnSiO3	another structure	another structure
FeSiO3	another structure	another structure
CoSiO3	another structure	another structure
NiSiO3	another structure	another structure
SmSiO3	another structure	X
MnSO3	another structure	another structure
FeSO3	another structure	another structure
TiTiO3	another structure	X
MnTiO3	another structure	X
FeTiO3	another structure	another structure
CoTiO3	another structure	another structure
NiTiO3	another structure	X
ZnTiO3	another structure	X
PdTiO3	another structure	X
HgTiO3	another structure	another structure
CrCrO3	another structure	another structure
MnGeO3	another structure	another structure
MnSeO3	another structure	X
MnPuO3	another structure	X
FeMoO3	another structure	another structure
CoGeO3	another structure	another structure
CoSeO3	another structure	another structure
CoUO3	another structure	X
NiSeO3	another structure	X
CuGeO3	another structure	X
CuSeO3	another structure	X
CuLaO3	another structure	X
CuTaO3	another structure	X
ZnSeO3	another structure	X
HgTeO3	another structure	X
BeO-ThO2	without compound ABO3	X
MgO-HfO2	without compound ABO3	X
Ti-W-O	without compound ABO3	X
PbO-PuO2	without compound ABO3	X

Table 3.9.2.2.21
ESTIMATION OF RESULTS OF EXAMINATION (Feature Set V)
Monoclinically Distorted Perovskite

Class of another structure :
number of objects - 39 ;
correctly - 19 [48.717949 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 20 [51.282051 %] ;

Class of without compound ABO3 :
number of objects - 4 ;
correctly - 0 [0 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 4 [100 %] ;

Number of objects - 43 ;
correctly - 19 [44.186047 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 24 [55.813953 %] ;

Table 3.9.2.2.22
Set for Examination (Feature Set IV)
Monoclinically Distorted Perovskite

Composition	Class	Result of examination
MnCO3	another structure	another structure
FeCO3	another structure	another structure
CoCO3	another structure	another structure
NiCO3	another structure	another structure
CuCO3	another structure	another structure
ZnCO3	another structure	another structure
SmCO3	another structure	perovskite mon.
YbCO3	another structure	X
RaCO3	another structure	X
MnSiO3	another structure	X
FeSiO3	another structure	another structure
CoSiO3	another structure	X
NiSiO3	another structure	X
SmSiO3	another structure	perovskite mon.
MnSO3	another structure	another structure
FeSO3	another structure	another structure
TiTiO3	another structure	perovskite mon.
MnTiO3	another structure	perovskite mon.
FeTiO3	another structure	X
CoTiO3	another structure	perovskite mon.
NiTiO3	another structure	perovskite mon.
ZnTiO3	another structure	X
PdTiO3	another structure	perovskite mon.
HgTiO3	another structure	perovskite mon.
CrCrO3	another structure	X
MnGeO3	another structure	X
MnSeO3	another structure	another structure
MnPuO3	another structure	another structure
FeMoO3	another structure	another structure
CoGeO3	another structure	X
CoSeO3	another structure	another structure
CoUO3	another structure	another structure
NiSeO3	another structure	another structure

Composition	Class	Result of examination
CuGeO3	another structure	another structure
CuSeO3	another structure	another structure
CuLaO3	another structure	another structure
CuTaO3	another structure	X
ZnSeO3	another structure	another structure
HgTeO3	another structure	perovskite mon.
BeO-ThO2	without compound ABO3	X
MgO-HfO2	without compound ABO3	X
Ti-W-O	without compound ABO3	perovskite mon.
PbO-PuO2	without compound ABO3	another structure

Table 3.9.2.2.23
ESTIMATION OF RESULTS OF EXAMINATION (Feature Set IV)
Monoclinically Distorted Perovskite

Class of another structure :
number of objects - 39 ;
correctly - 19 [48.717949 %] ;
incorrectly - 9 [23.076923 %] ;
indeterminately - 11 [28.205128 %] ;

Class of without compound ABO3 :
number of objects - 4 ;
correctly - 0 [0 %] ;
incorrectly - 2 [50 %] ;
indeterminately - 2 [50 %] ;

Number of objects - 43 ;
correctly - 19 [44.186047 %] ;
incorrectly - 11 [25.581395 %] ;
indeterminately - 13 [30.232558 %] ;

Table 3.9.2.2.24
Set for Examination (Feature Set V)
Rhombically Distorted Perovskite

Composition	Class	Result of examination
CaZrO3	perovskite rhomb.	X
CdVO3	perovskite rhomb.	X
SrPrO3	perovskite rhomb.	X
SrPbO3	perovskite rhomb.	X
BaCeO3	perovskite rhomb.	X
EuUO3	perovskite rhomb.	perovskite rhomb.
CoCO3	another structure	X
ZnCO3	another structure	X
SmCO3	another structure	X

Composition	Class	Result of examination
RaCO3	another structure	X
MgNbO3	another structure	without compound ABO3
MgCeO3	another structure	X
MnSiO3	another structure	X
NiSiO3	another structure	X
BaSiO3	another structure	X
PbSiO3	another structure	X
CdSO3	another structure	X
CaSnO3	another structure	X
CaThO3	another structure	X
FeTiO3	another structure	another structure
BaTiO3	another structure	X
PbTiO3	another structure	another structure
EuVO3	another structure	X
BaCrO3	another structure	X
CoMnO3	another structure	another structure
MnGeO3	another structure	another structure
SnMnO3	another structure	X
SrFeO3	another structure	X
BaFeO3	another structure	X
CoSnO3	another structure	X
SrNiO3	another structure	X
CuLaO3	another structure	X
SrGeO3	another structure	another structure
PbGeO3	another structure	another structure
SrMoO3	another structure	another structure
SrCeO3	another structure	X
SrAmO3	another structure	X
EuZrO3	another structure	X
BaRhO3	another structure	another structure
CdTeO3	another structure	another structure
CdThO3	another structure	X
SnPbO3	another structure	X
HgTeO3	another structure	another structure
BaIrO3	another structure	another structure
BaPuO3	another structure	X
EuHfO3	another structure	another structure
BeO-ZrO2	without compound ABO3	X
BeO-ThO2	without compound ABO3	X
MgO-PuO2	without compound ABO3	X
PbO-PuO2	without compound ABO3	X

Table 3.9.2.2.25
ESTIMATION OF RESULTS OF EXAMINATION (Feature Set V)
Rhombically Distorted Perovskite

Class of perovskite rhomb. :
number of objects - 6 ;
correctly - 1 [16.666667 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 5 [83.333333 %] ;

Class of another structure :
number of objects - 40 ;
correctly - 12 [30 %] ;
incorrectly - 1 [2.5 %] ;
indeterminately - 27 [67.5 %] ;

Class of without compound ABO3 :
number of objects - 4 ;
correctly - 0 [0 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 4 [100 %] ;

Number of objects - 50 ;
correctly - 13 [26 %] ;
incorrectly - 1 [2 %] ;
indeterminately - 36 [72 %] ;

Table 3.9.2.2.26
Set for Examination (Feature Set IV)
Rhombically Distorted Perovskite

Composition	Class	Result of examination
SrSnO3	perovskite rhomb.	X
SrUO3	perovskite rhomb.	perovskite rhomb.
BaThO3	perovskite rhomb.	X
CaCO3	another structure	another structure
CdCO3	another structure	another structure
YbCO3	another structure	another structure
MgSnO3	another structure	X
FeSiO3	another structure	another structure
CdSiO3	another structure	another structure
MnSO3	another structure	another structure
CaGeO3	another structure	another structure
CdTiO3	another structure	X
SrCrO3	another structure	X
NiMnO3	another structure	another structure
MnSnO3	another structure	X
CoGeO3	another structure	another structure
BaNiO3	another structure	X
ZnSnO3	another structure	another structure

Composition	Class	Result of examination
PbSeO3	another structure	X
EuNbO3	another structure	X
BaRuO3	another structure	X
BaSnO3	another structure	X
BaHfO3	another structure	X
BaPbO3	another structure	X
BaNpO3	another structure	another structure
PbIrO3	another structure	another structure
BeO-CeO2	without compound ABO3	X
MgO-RuO2	without compound ABO3	X

Table 3.9.2.2.27
ESTIMATION OF RESULTS OF EXAMINATION (Feature Set IV)
Rhombically Distorted Perovskite

Class of perovskite rhomb. :
number of objects - 3 ;
correctly - 1 [33.333333 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 2 [66.666667 %] ;

Class of another structure :
number of objects - 23 ;
correctly - 12 [52.173913 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 11 [47.826087 %] ;

Class of without compound ABO3 :
number of objects - 2 ;
correctly - 0 [0 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 2 [100 %] ;

Number of objects - 28 ;
correctly - 13 [46.428571 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 15 [53.571429 %] ;

Table 3.9.2.2.28
Set for Examination (Feature Set V)
Tetragonally Distorted Perovskite

Composition	Class	Result of examination
SrNiO3	another structure	X
SrNbO3	another structure	X
BaPbO3	another structure	X
CaVO3	another structure	another structure
BaThO3	another structure	X
CaMnO3	another structure	another structure
MnTeO3	another structure	X
SrIrO3	another structure	another structure
BaGeO3	another structure	X
PdTiO3	another structure	X
CoMnO3	another structure	X
SmCO3	another structure	X
SrPrO3	another structure	X
SrCrO3	another structure	X
CaZrO3	another structure	X
SrTiO3	another structure	X
SrMnO3	another structure	X
CuLaO3	another structure	X
SrOsO3	another structure	another structure
PbZrO3	another structure	another structure
CdCeO3	another structure	X
SrVO3	another structure	X
MnCO3	another structure	X
FeCO3	another structure	X
CdCO3	another structure	X
BaCO3	another structure	X
EuCO3	another structure	X
MgTiO3	another structure	another structure
FeTiO3	another structure	another structure
MgSnO3	another structure	X
SnMnO3	another structure	X
MgVO3	another structure	another structure
CaSiO3	another structure	another structure
PbSiO3	another structure	another structure
SnPbO3	another structure	X
CoCoO3	another structure	X
CoSiO3	another structure	another structure
CdSiO3	another structure	X
EuSiO3	another structure	another structure
FeSO3	another structure	another structure
BaCrO3	another structure	X
SrFeO3	another structure	X
CoUO3	another structure	X
CuSeO3	another structure	another structure
ZnSnO3	another structure	X
PbGeO3	another structure	X

Composition	Class	Result of examination
SrTeO3	another structure	X
CdTeO3	another structure	X
PbTeO3	another structure	another structure
PbIrO3	another structure	X
PbOsO3	another structure	X
BeO-PuO2	without compound ABO3	X
NiO-HfO2	without compound ABO3	X
MgO-HfO2	without compound ABO3	X
MgO-RuO2	without compound ABO3	X

Table 3.9.2.2.29
ESTIMATION OF RESULTS OF EXAMINATION (Feature Set V)
Tetragonally Distorted Perovskite

Class of another structure :
number of objects - 51 ;
correctly - 15 [29.411765 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 36 [70.588235 %] ;

Class of without compound ABO3 :
number of objects - 4 ;
correctly - 0 [0 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 4 [100 %] ;

Number of objects - 55 ;
correctly - 15 [27.272727 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 40 [72.727273 %] ;

Table 3.9.2.2.30
Set for Examination (Feature Set IV)
Tetragonally Distorted Perovskite

Composition	Class	Result of examination
CaCO3	another structure	another structure
CoCO3	another structure	another structure
NiCO3	another structure	another structure
CuCO3	another structure	another structure
ZnCO3	another structure	another structure
YbCO3	another structure	another structure
MnSiO3	another structure	another structure
FeSiO3	another structure	another structure
NiSiO3	another structure	another structure
SmSiO3	another structure	another structure

Composition	Class	Result of examination
MnSO3	another structure	another structure
CdSO3	another structure	another structure
CaMoO3	another structure	another structure
CaSnO3	another structure	another structure
CaIrO3	another structure	another structure
CaOsO3	another structure	another structure
CaPbO3	another structure	another structure
CaThO3	another structure	another structure
CaUO3	another structure	another structure
VVO3	another structure	another structure
CdVO3	another structure	another structure
MnMnO3	another structure	another structure
NiMnO3	another structure	another structure
ZnMnO3	another structure	another structure
MnGeO3	another structure	another structure
MnSeO3	another structure	another structure
MnPuO3	another structure	another structure
CoSnO3	another structure	another structure
CoTeO3	another structure	another structure
NiTeO3	another structure	another structure
CuGeO3	another structure	another structure
CuTeO3	another structure	another structure
CuTaO3	another structure	another structure
ZnTeO3	another structure	another structure
CdSeO3	another structure	another structure
CdSnO3	another structure	another structure
CdOsO3	another structure	another structure
CdPbO3	another structure	another structure
CdUO3	another structure	another structure
HgTeO3	another structure	another structure
LaLaO3	another structure	another structure
EuNpO3	another structure	another structure
BeO-ZrO2	without compound ABO3	without compound ABO3
BeO-UO2	without compound ABO3	without compound ABO3
MgO-UO2	without compound ABO3	without compound ABO3

Table 3.9.2.2.31
ESTIMATION OF RESULTS OF EXAMINATION (Feature Set IV)
Tetragonally Distorted Perovskite

Class of another structure :
number of objects - 42 ;
correctly - 42 [100 %] ;
incorrectly - 0 [0 %] ;
indeterminately - 0 [0 %] ;

```
Class of without compound ABO3 :
          number of objects - 3 ;
          correctly         - 3 [ 100 % ] ;
          incorrectly       - 0 [ 0 % ] ;
          indeterminately   - 0 [ 0 % ] ;

Number of objects           - 45 ;
          correctly         - 45 [ 100 % ] ;
          incorrectly       - 0 [ 0 % ] ;
          indeterminately   - 0 [ 0 % ] ;
```

The results of examination for feature set V testify that there is a vagueness of recognition which suggests that the level of the computer training is rather bad. A reliability of recognition in the case of the description in terms of the distribution of electrons in the shells of separate atoms, the ionic radii, and the corresponding formal valence (Feature set V) is less (on the average) than it is in the case of the description in terms of the type of incomplete electronic shell, electronegative, first, second, third, and fourth ionization potentials, standard entropies, Debye temperature, melting point, heat of melting, ionic radius, standard capacity, and formal valency. From the result obtained it may be deduced that the feature set IV is better for prediction of distortion type of crystal structure of compounds with composition $A^{II}B^{IV}O_3$ also.
The pyramidal networks and the corresponding logical expressions were formed as a result of the computer learning via CONFOR. Appendix 11 contains the logical expressions for various learning sets and for various types of symmetry.

The table of predictions of the crystal structure type for the compounds of composition $A^{I}B^{V}O_3$ (Table 3.9.2.2.32) results from comparison of the results of predicting the crystal structure type and distortion type with use of the descriptions in terms of the Features Sets IV, V, VIII (see Section 2.6.3). The designations see in Section 3.9.2.1.3.

The physical-chemical systems, which were investigated experimentally, were outlined by double lines. The empty square corresponds to the lack of coincidence of the predictions, which have been obtained using different feature sets.

The analysis of Table 3.9.2.2.32 shows: the great number of predictions of new compounds with crystal structure type of cubic, rhombic and monoclinic perovskite, were obtained.

Table 3.9.2.2.32
Table of Predictions of Crystal Structure Type
for Compounds of Composition $A^{II}B^{IV}O_3$

A / B	Be	Mg	Ca	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ge	Sr	Tc	Ru	Pd	Ag	Cd	Sn	Ba	La	Sm	Eu	Yb	Hg	Pb	Ra
C		C	C		?	?	C	C	C	C	C	C		A		?	?		C	?	A	?	A	A	A		A	A
Si		-	-	?	*	-	-	-	-	?	?	?		-	?	?	?		?		-	?	-	-	?	?	-	?
S			?		-	-	-	-	-	?	P	?		?		?	?		-	I	-	?	?	?	-		-	?
Ti		I	2,4	-	-	?	I	I	I	I	?	I		1					I	?	15	?	P	1	4	L	5	L
V	C	-	1,2		-	?	I		-	?	P	I		1					2	I		?	P	4	2			
Cr	C	?	2			-	I	-	?	?	-	?	?	1					?		?					?	1	?
Mn			124		I		-		I	I	?	?		3					?	I	3						P	
Fe			?					-			?	?		?					?		3,5					?	?	?
Co		?	?						-		?	?		1					?		3					?	?	?
Ni			P							-	?	P		3					P		3					?	?	?
Ge		-	-			?	-		-	?	?	?		-					-	?	-		?	?			-	
Se	*	2	?	?	?	?	2	P	2	2	2	2		?	P				?	?	?	?	?	?	?		-	?
Zr	*		2,4	?			?	*	-			124		2		P			4		1	?		1			2	P
Nb		I	2,4		?	?	-	I	?				1	3					?		1	?	?	1	?		-	
Mo			2			-	-	-	-				?	1	*	*		?	P		1	?	P	?	2			P
Tc	*		2						-		P	?		1					?	?	1,3							
Ru	*	*	1,2											124			*		?		3	12		?		?	2	
Rh	*										?			3	*		*				?					-	-	?

A / B	Be	Mg	Ca	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ge	Sr	Tc	Ru	Pd	Ag	Cd	Sn	Ba	La	Sm	Eu	Yb	Hg	Pb	Ra
Pd	*			?	?				?	?	?			?	*	*					?	?				?		?
Sn		I	I			?	I		-		P	P		124		?	?	124	-		1	P	P	P		-	-	P
Te	*	2	?			-	2		2	?	2	?		?		?	?	2,4	-	P	-	-	4	1		-	-	
La		?	?								3			?					?		?	-				?	-	?
Ce	*	14	1,4		*						P	?		4,5					14		1245					14	1
Pr	*	*	1,4								P	I		2					24		124		*	*			
Tb	*	*									P	I		2					4		2,3		*	*	?		
Hf	*	*	4					*		*	P	?		124		2			2		1		?	1		P	P
Ta			?								P		?	?		?	?		?	P	4,5		?	?	?		
W	*		?	*	*				-	?	?		?	?			?		?	2	1						P
Re	*		?		*	?					P			?	?	?			?	2			?	?	?		
Os	*		2	?		?	?	?	?		P	2		2	P		?		2	P	3		P	?	P		-	p
Ir	*		2	?	*	?	?	?	?	4	?	?	?	4					4	P	3,4		P	?	P	?	-	?
Pt	*		2,4		*						P	?		4	*				4	12	3							
Pb	*		I								P	?		2,4					I	-	1,4					?		
Po			?	-	-	?	-	?	?	?	?	?	-	?	?				?	I	-		?	?	-	-		
Th	*	1	1,4	?					-		4	?		1,4			?		14	?	1,2		?	?				
Pa	*	*				?			-		P	I		134			?		4		1		?	?	?			
U	*	*	1,2			?			-	?	2	I		2,3					P		1	?	P	2	?			
Np	*	*	1		*				-		2	?		2,3					?		1	?		2				
Pu	*	*	?		*		2	I	-		2	?		1234					?		1	?		2			*	

A / B	Be	Mg	Ca	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ge	Sr	Tc	Ru	Pd	Ag	Cd	Sn	Ba	La	Sm	Eu	Yb	Hg	Pb	Ra
Am	*	*	1,4			-			-		P	I		1					4		1		?	?	?			
Cm	*	*	1,4		-	-	-	-	-	P	2	I	-	234					P	I	1	-	?	?	?	-		
Bk	*	*	1,4		-	-	-	-	-	P	2	I	-	234					P	I	?	-	?	?	?	-		
Cf	*	*	1,4		-	-	-	-	-	P	2	I	-	234					P	I	1	-	?	?	?	-		

3.9.2.2.6. Analyse of Semantic Networks and Corresponding Logical Expressions

Table 3.9.2.2.33 contains the results of analyse for various classes and for description of elements A_{II} and B_{IV} in terms of feature set IV.

Table 3.9.2.2.33
Result of Analyse of Pyramidal Network (Feature Set IV)
(Prediction of Crystal Structure Type)

Conjunction	Number of recurrences
Perovskite	
I12, I21	44
R10, TD2	40
E2, TM4	39
R10, S	36
I12, I21, R10, TD2	35
I21, C7	29
TD2, C7	28
I12, I21, C7	28
S, H3	27
I21, S7	23
C7, S8	23
TD2, C7, S8	23
TD2, S8	23
I21, S7, C8	21
I12, I21, E2, TM4, C7	21
I12, I21, I46	21
I21, S, S7, C8	20
S, H4	20
H3, D	20
Calcite	
E10, TD1	8
P, C1	8
I310, I49	8
R1, S1	8
P, C1, R1, S1	8
P, C1, I310, I49, R1, S1	8
P, C1, I310, I49, R1, S1, I111, I29	8
E10, TD11, P, C1, I310, I49, R1, S1, I111, I29	8
TD11, C1	8
TD11, C1, R1, S1	8
Ilmenite	
D, H6	11
I16, I24	10
D, H6, I47	10

Analyse of Table 3.9.2.2.33 shows that the fields of structure types of compounds with composition $A^{II}B^{IV}O_3$ don't intersect in the multi-dimensional space of feature set IV.

Table 3.9.2.2.34 contains the results of analyse for various classes and for description of compounds in terms of feature set VIII.

Table 3.9.2.2.34
Result of Analyse of Pyramidal Network (Feature Set VIII)
(Prediction of Crystal Structure Type)

Conjunction	Number of recurrences
Perovskite	
V2, V4, H7	62
V2, V4, C3	47
V2, V4, H7, TM8	46
V2, V4, TM6	36
V2, V4, H7, TM8, R11	35
V2, V4, C2	27
C3, TM6	26
V2, V4, C3, TM6	26
V2, TM4	25
V2, V4, TM6, R12	25
V2, V4, H7, R12	23
V2, V4, H7, TM6, R12	23
V2, V4, H7, C3, TM6, R12	23
V2, V4, H3	23
V2, V4, H7, C3, TM8, R11	22
Calcite	
H5, TM1	9
H5, TM1, R1	9
H5, TM1, R1, C1	9
V2, V4, H5, TM1, R1, C1	9
Ilmenite	
V2, V4, TM6	11
V2, V4, R6	11
TM6, C4	9
V2, V4, TM6, C4	9
TM6, C4, R2	8

Analyse of Table 3.9.2.2.34 shows that the fields of structure types of compounds with composition $A^{II}B^{IV}O_3$ don't intersect in the multi-dimensional space of feature set of simple oxides.

4. SEARCH FOR CORRELATIONS BETWEEN T_C AND THE PROPERTIES OF HTSC COMPONENTS

The great number of synthesized high temperature superconductors (HTSC) can be classified schematically under 6 classes [83]:

- $La_{2-x}M_xCuO_{4-\pi}$(M - Ca, Sr or éá);
- (Ln, Ln`)(Ba, M)$_2$(Cu, M`)$3O_{7+-\pi}$;
- two groups of the thallic and bismuthic phases with alkaline--earth metals and copper;
- cubic perovskites without copper of $M_\sigma Ba_{1-\sigma}BiO_3$ type;
- various types of T-phases.

So hundreds of already known HTSC represent the products of substitution of one or another component of "basic" compound. The choice of a doped component usually depends on the theoretical conceptions of the investigator, his experience and intuition. In order to find the most important correlations between T_C (critical temperature of transition to superconducting state) and the component properties the statistical analysis of data about several groups of superconducting oxide phases had been done. The results of correlation analysis will help to make the target-oriented search for new HTSC of the types described. Such a statistical correlation analysis helped us [84] to find the interdependences between T_C, component properties and the unit cell parametres of Chevrel phases with selenium.

The problem of search for correlation between T_C and other compound properties is divided into three parts: the analysis of dependence between T_C and composition of certain composition (in other words the analysis of the diagram "composition - property"); the examination of dependences between T_C and the conditions of synthesis of superconducting phases of fixed composition; finding of correlations between T_C and the component properties of well-known phases. The last problem (in contradiction with first two, solved in order to find the T_C correlations of the certain phase) reveals the tendency of some set of phases to have the superconducting properties.

The physico-chemical analysis of T_C-dependence upon the composition and the search for optimal synthesis conditions maximising the phases T_C are usual during the deep investigation of HTSC. That's why the number of works devoted to the finding correlations between T_C, the composition of phases and their synthesis conditions are so great. Only several articles [85-89] are devoted to the search for dependence between T_C and component properties. The analysis of T_C dependence of the compounds with $YBa_2Cu_3Ç_zO_{7-x}$ composition upon the ionic radius of alkaline or alkaline-earth metal A showed the linear dependence between these quantities and also between T_C and first ionization po-

tential of doped element [85]. The correlation between T_c of HTSC and the difference [86,87] or more complicated function [88] of electronegativity of cations and anions, and also its effective charge [87] have been found. It was the attempt to construct the complicated empirical exponential criterion including size factors for different crystal structures, which practically linear correlate with T_c [89].

4.1. Description of Method

In this work we have found the statistically significant correlations between T_c, concentration and the properties of components of "1-2-3" phases and different types of T-phases.

D-r L.V.Molchanova from Moscow State University rendered assistance in data collection. The information for the computer learning was assessed by expert on HTSC Dr.E.V.Antipov (Moscow State University).

Sampling coefficient of linear correlation between T_c and property x_j was calculated in accordance with a formula:

$$r = \frac{\sum_{i=1}^{N} (x_{ji} - x_{mj}) * (Æ_{ci} - Æ_{cm})}{\left(\sum_{i=1}^{N} (x_{ji} - x_{mj}) * \sum_{i=1}^{N} (Æ_{ci} - Æ_{cm})\right)^{1/2}},$$

where N - is the number of phases of certain type;
$i = 1, \ldots, N$;
$j = 1, \ldots, M$;
M - is the number of properties under examination;
σ_{mj} and $Æ_{cm}$ - mean arithmetical of σ_j and $Æ_c$.

The interdependence between Tk and the components properties is considered to be important if the absolute value of calculated correlation coefficient is more than some fixed table value of confidence level alpha = 0.05. The positive value of correlation coefficient testifies that x_j increasing leads to the increasing of T_c. On the opposite, the negative value testifies that x_j increasing leads to the decreasing T_c.

It's supposed . that any mutual distribution of random variables T_c and x_j is normal.

4.2. The compounds of (Ln, Ln`)(Ba, M)$_2$ (Cu,M`)$3O7+-y$ composition

The set for analysis included the data about 286 phases of a composition described (Table 4.2.1).

Table 4.2.1

Phases of composition $(Ln, Ln`)(Ba,M)_2 (Cu,M`)_3O_{7+-y}$

N	Composition	T_c, K
1	YBa Cu O 2 3 6.38	60
2	YBa Cu O 2 3 6.89	90
3	YBa Cu O 2 3 6.97	94
4	YBa Cu O 2 3 6.25	0
5	YBa Cu O 2 3 6.6	46
6	YBa Cu O 2 3 6.8	91.6
7	YBa Cu O 2 3 6.77	91
8	YBa Cu O 2 3 6.7	70
9	YBa Cu O 2 3 6.53	56
10	YBa Cu O 2 3 6.3	0
11	YBa Cu O 2 3 6.95	91
12	YBa Cu O 2 3 6.9	89.6
13	LaBa Cu O 2 3 7	90
14	La Ba Cu O 1.2 1.8 3 6.9	60
15	La Ba Cu O 1.3 1.7 3 7	50
16	LaBa Cu O 2 3 6.8	72
17	LaBa Cu O 2 3 6.4	0
18	LaBa Cu O 2 3 6.6	42
19	LaBa Cu O 2 3 7	70
20	PrBa Cu O 2 3 7	0
21	NdBa Cu O 2 3 7	84
22	Nd Ba Cu O 1.35 1.65 3 7	0

N	Composition	T_c, K
23	$SmBa_2Cu_3O_7$	94.2
24	$EuBa_2Cu_3O_7$	93.5
25	$Eu_{1.2}Ba_{1.8}Cu_3O_{7.18}$	28
26	$EuBa_2Cu_3O_{6.9}$	90
27	$EuBa_2Cu_3O_{6.47}$	0
28	$EuBa_2Cu_3O_{6.35}$	0
29	$EuBa_2Cu_3O_{6.25}$	0
30	$GdBa_2Cu_3O_7$	92
31	$GdBa_2Cu_3O_{6.86}$	90
32	$DyBa_2Cu_3O_7$	92
33	$DyBa_2Cu_3O_{6.82}$	91
34	$DyBa_2Cu_3O_7$	87.1
35	$HoBa_2Cu_3O_7$	93
36	$ErBa_2Cu_3O_7$	92.7
37	$ErBa_2Cu_3O_7$	90
38	$ErBa_2Cu_3O_{6.6}$	65
39	$ErBa_2Cu_3O_{6.7}$	68
40	$TmBa_2Cu_3O_7$	86
41	$TmBa_2Cu_3O_{6.6}$	56
42	$YbBa_2Cu_3O_{6.85}$	90
43	$YbBa_2Cu_3O_{6.95}$	88.7
44	$LuBa_2Cu_3O_7$	84
45	$Y_{0.9}Ca_{0.1}Ba_2Cu_3O_{6.98}$	88
46	$Y_{0.8}Ca_{0.2}Ba_2Cu_3O_{6.98}$	76

N	Composition	T , K c
47	Y Ca Ba Cu O 0.8 0.2 2 3 6.2	84
48	Y La Ba Cu O 0.5 0.5 2 3 7	82
49	Y Pr Ba Cu O 0.9 0.1 2 3 7	89
50	Y Pr Ba Cu O 0.5 0.5 2 3 7	25.4
51	Y Eu Ba Cu O 0.5 0.5 2 3 7	92
52	Y Gd Ba Cu O 0.9 0.1 2 3 6.88	91.5
53	Y Gd Ba Cu O 0.7 0.3 2 3 6.99	91
54	Y Gd Ba Cu O 0.5 0.5 2 3 6.9	91
55	Y Tb Ba Cu O 0.84 0.16 2 3 7	92
56	Y Dy Ba Cu O 0.9 0.1 2 3 6.98	92
57	Y Dy Ba Cu O 0.7 0.3 2 3 6.96	92
58	Y Dy Ba Cu O 0.5 0.5 2 3 6.9	91
59	Y Er Ba Sr Cu O 0.9 0.1 1.9 0.1 3 7	88
60	Y Er Ba Cu O 0.5 0.5 2 3 7	90
61	Y Lu Ba Cu O 0.938 0.062 2 3 7	93.2
62	Y Lu Ba Cu O 0.75 0.25 2 3 7	91.7
63	Y Ca Ba La Cu O 0.5 0.5 1.5 0.5 3 6.8 8	82
64	Eu Pr Ba Cu O 0.75 0.25 2 3 7	0
65	Eu Y Ba Cu O 0.9 0.1 2 3 7	93.7
66	Eu Y Ba Cu O 0.75 0.25 2 3 7	95
67	Eu Pr Ba Cu O 0.9 0.1 2 3 7	80
68	Gd Y Ba Cu O 0.9 0.1 2 3 7	90
69	Gd Y Ba Cu O 0.7 0.3 2 3 6.95	90
70	Gd Y Ba Cu O 0.9 0.1 2 3 6.9	90.5

N	Composition	T , K c
71	Gd Eu Ba Cu O 0.6 0.4 2 3 7	74
72	Dy Y Ba Cu O 0.7 0.3 2 3 6.85	90.5
73	Dy Y Ba Cu O 0.9 0.1 2 3 6.92	91
74	YBa Cu Ti O 2 2.7 0.3 7	75
75	YBa Cu Ti O 2 2.997 0.03 7	92
76	YBa Cu Al O 2 2.8 0.2 7.15	71.6
77	YBa Cu Al O 2 2.9 0.1 7.1	68
78	YBa Cu Al O 2 2.9 0.1 7.25	86
79	YBa Cu Al O 2 2.7 0.3 7	55
80	YBa Cu Al O 2 2.7 0.3 7.2	82
81	YBa Cu Al O 2 2.5 0.5 7	50
82	YBa Cu Al O 2 2.9 0.1 7	77
83	YBa Cu Cr O 2 2.7 0.3 7	84.5
84	YBa Cu Mn O 2 2.7 0.3 7	78.9
85	YBa Cu Mn O 2 2.4 0.6 7	78
86	YBa Cu Mn O 2 2.775 0.225 7	89
87	YBa Cu Mn O 2 2.55 0.45 7	72
88	YBa Cu Fe O 2 2.65 0.35 7	0
89	YBa Cu Fe O 2 2.5 0.5 7.2	0
90	YBa Cu Fe O 2 2.7 0.3 7	38
91	YBa Cu Fe O 2 2.91 0.09 7	90
92	YBa Cu Fe O 2 2.82 0.18 7	55
93	YBa Cu Fe O 2 2.875 0.125 7	43
94	YBa Cu Fe O 2 2.94 0.06 7	76

N	Composition	T_c, K
95	YBa Cu Co O 2 2.7 0.3 7	21.2
96	YBa Cu Co O 2 2.6 0.4 7.32	0
97	YBa Cu Ni O 2 2.9 0.1 6.7	82
98	YBa Cu Ni O 2 2.9 0.1 6.8	87
99	YBa Cu Ni O 2 2.8 0.2 6.6	75
100	YBa Cu Ni O 2 2.8 0.2 6.6	85
101	YBa Cu Ni O 2 2.7 0.3 6.5	72
102	YBa Cu Ni O 2 2.7 0.3 6.8	85
103	YBa Cu Ni O 2 2.5 0.5 6.4	62
104	YBa Cu Ni O 2 2.5 0.5 6.8	84
105	YBa Cu Ni O 2 2.64 0.36 7	40
106	YBa Cu Ni O 2 2.7 0.3 7	66.3
107	YBa Cu Fe O 2 2.88 0.12 7	81
108	YBa Cu Zn O 2 2.7 0.3 6.9	0
109	YBa Cu Zn O 2 2.7 0.3 7	0
110	YBa Cu Zn O 2 2.95 0.05 6.9	84
111	YBa Cu Zn O 2 2.95 0.05 6.8	73
112	YBa Cu Zn O 2 2.9 0.1 6.6	58
113	YBa Cu Zn O 2 2.9 0.1 6.9	83
114	YBa Cu Zn O 2 2.85 0.15 6.5	58
115	YBa Cu Zn O 2 2.8 0.2 6.6	58
116	YBa Cu Zn O 2 2.8 0.2 6.9	80
117	YBa Cu Zn O 2 2.85 0.15 6.9	80
118	YBa Cu Zn O 2 2.7 0.3 6.4	47

N	Composition	T , K c
119	YBa Cu Zn O 2 2.7 0.3 6.9	81
120	YBa Cu Zn O 2 2.9 0.1 7	54.3
121	YBa Cu Ga O 2 2.97 0.03 7	90
122	YBa Cu Ga O 2 2.7 0.3 7	25
123	YBa Cu Pd O 2 2.997 0.003 7	94
124	YBa Cu Ag O 2 2.997 0.003 7	94
125	YBa Cu Sn O 2 2.9 0.1 6.8	83
126	YBa Cu Sn O 2 2.7 0.3 7.35	87
127	YBa Cu Sn O 2 2.9 0.1 7.3	79
128	YBa Cu Sn O 2 2.8 0.2 7.34	86
129	NdBa Cu Ni O 2 2.9 0.1 7	70.9
130	NdBa Cu Zn O 2 2.9 0.1 7	36.9
131	EuBa Cu Zn O 2 2.7 0.3 7	0
132	EuBa Cu Sn O 2 2.97 0.03 6.9	89
133	EuBa Cu Sn O 2 2.91 0.09 7	86
134	EuBa Cu Sn O 2 2.85 0.15 6.8	87
135	EuBa Cu Sn O 2 2.76 0.24 6.8	86
136	GdBa Cu Sn O 2 2.97 0.03 7	90
137	GdBa Cu Zn O 2 2.9 0.1 7	53.6
138	DyBa Cu Zn O 2 2.9 0.1 7	49.3
139	ErBa Cu Zn O 2 2.9 0.1 7	51.8
140	YBa Ca Cu O 1.95 0.05 3 6.8	85
141	YBa Ca Cu O 1.95 0.05 3 7	88
142	YBa Ca Cu O 1.9 0.1 3 6.8	84

N	Composition	T , K c
143	YBa Ca Cu O 1.85 0.15 3 6.8	84
144	YBa Ca Cu O 1.85 0.15 3 6.9	86
145	YBa Ca Cu O 1.8 0.2 3 6.6	81
146	YBa Ca Cu O 1.8 0.2 3 6.9	86
147	YBa Sr Cu O 1.5 0.5 3 7	86
148	YBa Sr Cu O 1.9 0.1 3 6.9	86
149	YBa Sr Cu O 1.9 0.1 3 7	88
150	YBa Sr Cu O 1.7 0.3 3 6.9	86
151	YBa Sr Cu O 1.7 0.3 3 7	87
152	YBa Sr Cu O 1.5 0.5 3 6.9	86
153	YBa Sr Cu O 1.5 0.5 3 6.8	84
154	YBa Sr Cu O 1.3 0.7 3 6.7	81
155	YBa Sr Cu O 1.3 0.7 3 6.9	86
156	YBa Sr Cu O 1.1 0.9 3 6.6	80
157	YBa Sr Cu O 1.1 0.9 3 6.9	86
158	YBa La Cu O 1.7 0.3 3 7	82
159	YBa La Cu O 1.5 0.5 3 7	20
160	YBa La Cu O 1.4 0.6 3 7	0
161	LaBaCaCu O 3 7	77.8
162	LaBaCaCu O 3 6.85	77
163	LaBaSrCu O 3 6.5	33
164	LaBaSrCu O 3 6.3	0
165	EuBa Eu Cu O 1.9 0.1 3 7	60
166	EuBa Eu Cu O 1.8 0.2 3 7	40

N	Composition	T , K c
167	GdBa Sr Cu O 1.5 0.5 3 7	77
168	YBa K Cu O 1.9 0.1 3 7	93
169	Y Ho Ba Cu O 0.9 0.1 2 3 6.95	89
170	YBa Ca Cu O 1.5 0.5 3 7	82
171	YBaCaCu O 3 7	80
172	YBa Cu Zn O 2 2.9 0.1 6.94	57
173	YBa Ca Cu O 1.9 0.1 3 6.84	85
174	YBa Sr Cu O 1.9 0.1 3 6.89	89
175	YBa Cu Ni O 2 2.95 0.05 7	86.8
176	NdBa Cu Ni O 2 2.95 0.05 7	85
177	NdBa Cu Zn O 2 2.95 0.05 7	65
178	GdBa Cu Ni O 2 2.95 0.05 7	86.2
179	GdBa Cu Ni O 2 2.9 0.1 7	84.5
180	GdBa Cu Zn O 2 2.95 0.05 7	72.5
181	DyBa Cu Ni O 2 2.95 0.05 7	87.5
182	DyBa Cu Ni O 2 2.9 0.1 7	81.8
183	DyBa Cu Zn O 2 2.95 0.05 7	71.5
184	ErBa Cu Ni O 2 2.95 0.05 7	87.8
185	ErBa Cu Ni O 2 2.9 0.1 7	83.3
186	ErBa Cu Zn O 2 2.95 0.05 7	73.1
187	YBa Sr Cu O 1.48 0.52 3 7	95
188	YBaSrCu O 3 7	86
189	YBa Ca Cu O 1.25 0.75 3 7	85
190	EuBa Ca Cu O 1.85 0.15 3 7	78

N	Composition	T , K c
191	EuBa Ca Cu O 1.5 0.5 3 7	64
192	EuBa Ca Cu O 1.25 0.75 3 7	44
193	GdBa Sr Cu O 1.8 0.2 3 7	90
194	GdBa Sr Cu O 1.6 0.4 3 7	88
195	GdBa Sr Cu O 1.4 0.6 3 7	77
196	Y Eu Ba Cu O 0.8 0.2 2 3 6.95	88
197	Y Dy Ba Cu O 0.8 0.2 2 3 6.95	89
198	Y Sm Ba Cu O 0.8 0.2 2 3 6.95	91
199	Y Yb Ba Cu O 0.8 0.2 2 3 6.95	93
200	Y Tb Ba Cu O 0.8 0.2 2 3 6.95	94
201	YBa Cu Fe O 2 2.99 0.01 6.95	93
202	YBa Cu Fe O 2 2.98 0.02 6.95	92
203	YBa Cu Fe O 2 2.97 0.03 6.95	89
204	YBa Cu Fe O 2 2.95 0.05 6.95	84
205	YBa Cu Fe O 2 2.9 0.1 6.95	68
206	YBa Cu Al O 2 2.99 0.01 6.95	93
207	YBa Cu Al O 2 2.98 0.02 6.95	89
208	YBa Cu Al O 2 2.97 0.03 6.95	88
209	YBa Cu Al O 2 2.95 0.05 6.95	84
210	YBa Cu Al O 2 2.9 0.1 6.95	85
211	YBa Cu Zn O 2 2.99 0.01 6.95	84
212	YBa Cu Zn O 2 2.97 0.03 6.95	62
213	YBa Cu Zn O 2 2.95 0.05 6.95	41
214	YBa Cu Zn O 2 2.9 0.1 6.95	25

N	Composition	T_c, K
215	YBa Cu Zn O 2 2.99 0.01 6.95	82
216	YBa Cu Zn O 2 2.98 0.02 6.95	80
217	YBa Cu Zn O 2 2.97 0.03 6.95	71
218	YBa Cu Zn O 2 2.95 0.05 6.95	76
219	YBa Cu Zn O 2 2.9 0.1 6.95	51
220	YBa Cu Co O 2 2.9 0.1 7	74
221	YBa Cu Co O 2 2.833 0.167 7	55
222	YBa Cu Co O 2 2.75 0.25 7	26
223	YBa Cu Ni O 2 2.75 0.25 7	64
224	YBa Cu Ni O 2 2.5 0.5 7	52
225	YBa Cu Al O 2 2.97 0.03 7	91
226	YBa Cu Al O 2 2.94 0.06 7	92
227	YBa Cu Al O 2 2.895 0.105 7	99
228	YBa Cu Al O 2 2.862 0.138 7	102
229	YBa Cu Al O 2 2.85 0.15 7	99
230	YBa Cu Al O 2 2.711 0.289 7	93
231	YBa Cu Al O 2 2.58 0.42 7	82.5
232	YBa Cu Al O 2 2.975 0.025 7	83
233	YBa Cu Al O 2 2.95 0.05 7	75
234	YBa Cu Al O 2 2.925 0.075 7	65
235	YBa Cu Ti O 2 2.985 0.015 7	90
236	YBa Cu Ti O 2 2.95 0.05 7	88
237	YBa Cu Ti O 2 2.9 0.1 7	91
238	YBa Cu Ti O 2 2.87 0.13 7	92

N	Composition	T , K c
239	YBa Cu Ti O 2 2.8 0.2 7	93
240	YBa Cu Fe O 2 2.99 0.01 7	91
241	YBa Cu Fe O 2 2.98 0.02 7	89
242	YBa Cu Fe O 2 2.96 0.04 7	77
243	YBa Sr Cu O 1.75 0.25 3 7	90
244	YBa Sr Cu O 1.25 0.75 3 7	85
245	YBa Ca Cu O 1.75 0.25 3 7	86.5
246	Y Lu Ba Cu O 0.5 0.5 2 3 7	93.5
247	Y La Ba Cu O 0.75 0.25 2 3 7	87.5
248	Y La Ba Sr Cu O 0.85 0.15 1.75 0.25 3 7	87
249	Y In Ba Cu O 0.75 0.25 2 3 7	90
250	Y Zr Ba Cu O 0.9 0.1 2 3 7	93.5
251	YBa La Cu O 1.75 0.25 3 7	96
252	La Ca BaLaCu O 0.5 0.5 3 7	70
253	Gd Pr Ba Cu O 0.51 0.49 2 3 7	0
254	LaBaPrCu O 3 7	0
255	Y Sm Ba Cu O 0.9 0.1 2 3 7	88
256	Eu Gd Ba Cu O 0.8 0.2 2 3 7	44
257	Eu Gd Ba Cu O 0.75 0.25 2 3 7	91
258	Y Yb Ba Cu O 0.85 0.15 2 3 7	91
259	YBaSrCu O 3 6.9	81
260	Y Bi Ba Cu O 0.97 0.03 2 3 7	105
261	Y Bi Ba Cu O 0.9 0.1 2 3 7	100
262	Y Ca Ba Cu O 0.6 0.4 2 3 7	80

N	Composition	T_c, K
263	Y Ca Ba Cu O 0.2 0.8 2 3 7	70
264	YBa Cu Zn O 2 2.975 0.025 7	82
265	YBa Cu Zn O 2 2.925 0.075 7	65
266	YBa Cu Zn O 2 2.8 0.2 7	54
267	YBa Cu Zn O 2 2.7 0.3 7	47
268	YBa Cu Ni O 2 2.975 0.025 7	87
269	YBa Cu Ni O 2 2.95 0.05 7	85
270	YBa Cu Ni O 2 2.925 0.075 7	82
271	YBa Cu Ni O 2 2.75 0.25 7	74
272	YBa Cu Al O 2 2.8 0.2 7	71.6
273	YBa Cu Al O 2 2.75 0.25 7	58
274	YBa Cu Sn O 2 2.95 0.05 7	90.1
275	YBa Cu Sn O 2 2.7 0.3 7	89
276	YBa Ca Cu O 1.925 0.075 3 7	86
277	Y Pr Ba Cu O 0.7 0.3 2 3 7	49
278	Pr Pr Ba Cu O .0.7 0.3 2 3 7	0
279	LaCaBaCu O 3 6.88	78
280	LaCaBaCu O 3 6.86	70
281	LaCaBaCu O 3 6.84	60
282	LaCaBaCu O 3 6.83	45
283	LaCaBaCu O 3 6.79	33
284	LaCaBaCu O 3 6.76	30
285	LaCaBaCu O 3 6.71	12
286	LaCaBaCu O 3 6.69	12

Here and further the element properties were taken from [90], ionic radii - from [91]. The coefficients of linear correlation of T_c with the following properties were calculated: concentration of Ln, Ln`, Ba, M, M`, and O, first three potentials of ionization, ionic radius of corresponding cations, the number of electrons in the incomplete d- and f- shells, electronegatives by Pauling, standard entropies of individual substance, standard isobaric thermal capacities, temperature and heat of melting and boiling, Debye temperature of elements Ln, Ln`, M and M`.

The critical value of coefficient of linear corellation equals 0.12 [92] for the degree of freedom f = N - 2 = 284 and the confidence level alpha = 0.05. Table 4.2.2 gives the properties most influencing on T_c with such a critical value of linear correlation coefficient.

Table 4.2.2
The component properties of phases with composition $(Ln,Ln`)(Ba,M)_2(Cu,M`)_3O_{7+-\pi}$ most influencing on T_c

Property	The value of correlation coefficient
concentration of é	0.1756
concentration of î	- 0.1795
concentration of M`	- 0.2004
concentration of Ä	0.3023
1-st potential of ionization of Ln	0.3461
2-nd potential of ionization of Ln	0.3137
ionic radius of Ln	- 0.2363
electronegativity of Ln	0.2183
standard entropies of individual substance Ln	- 0.1612
melting temperature of Ln	0.3290
heat of melting Ln	0.3341
Debye temperature of Ln	0.2470
1-st potential of ionization of Ln`	0.3367
2-nd potential of ionization of Ln`	0.2435
ionic radius of Ln`	- 0.2002
electronegativity of Ln`	0.1348
melting temperature of Ln`	0.1916
boiling temperature of Ln`	- 0.1209
heat of melting of Ln`	0.2182
Debye temperature of Ln`	0.1239
3-rd potential of ionization of M	0.1283
ionic radius of î	0.1740
the number of electrons on the incomplete f-shell of î	- 0.1918
elecronegativity of î	- 0.1463
melting temperature of î	- 0.1641
boiling temperature of î	- 0.1743

Property	The value of correlation coefficient
heat of melting of î	- 0.1425
heat of boiling of î	- 0.1695
1-st potential of ionization of M`	- 0.2253
3-rd potential of ionization of M`	- 0.1745
boiling temperature of î`	- 0.2016
heat of boiling of î`	0.1491

The most influential properties are the first ionization potentials of lanthanides.Their increasing leads to the growth of temperature of transition to superconducting state of "1-2-3" compounds. According to the majority of experimental data the oxygen concentration in these phases is also one of the most influential properties. It's increasing (within some boundaries) leads to the growth of critical temperature of transition to superconducting state. The tendency of T_c to grow may be also a result of: increasing of barium concentration; values of the second potentials of ionization; temperatures and heats of melting; electronegativity and Debye temperature of Ln and Ln` components; third potential of ionization and ionic radius of M component; heat of boiling of M` component. The cause of T_c decrease is the following: growth of concentration of basic M and doped M` component; ionic radii of Ln and Ln`; standard entropy of Ln; boiling temperature of Ln; the number of electrons on incomplete f-shell and electronegativity of M component, it's temperature and heat of melting and boiling; the first and the third potential of ionization of M'-doped component and it's boiling temperature.

4.3. T-phases of $(La,Ln,Sr)_2 CuO_4$ composition

The sample included the data about 44 phases (Table 4.3.1). The correlation coefficients of T_c with the following properties were calculated: concentration of Ln and Sr and also with all the properties of Ln component analysed for the previous class of phases.

Table 4.3.1
T-Phases of composition $(La,Ln,Sr)_2CuO_4$

N	Composition, C.N.= 9	T_c, K
1	La Yb Sr CuO 1.8 0.05 0.15 4	36
2	La Yb Sr CuO 1.85 0.1 0.05 4	34
3	La Sr CuO 1.85 0.15 4	38
4	La Sr CuO 1.7 0.4 4	0

N	Composition, C.N.= 9	T , K c
5	La Eu Sr CuO 1.6 0.25 0.15 4	17
6	La Ba CuO 1.8 0.2 4	30
7	La Ba CuO 1.85 0.15 4	30
8	La Nd Sr CuO 1.82 0.03 0.15 4	34.2
9	La CuO 2 4	37
10	La Sr CuO 1.9 0.1 4	40
11	La Nd Sr CuO 1.45 0.4 0.15 4	22.5
12	La Pr Sr CuO 1.7 0.15 0.15 4	32
13	La Nd Sr CuO 1.7 0.15 0.15 4	28
14	La Sm Sr CuO 1.7 0.15 0.15 4	14
15	La Eu Sr CuO 1.7 0.15 0.15 4	21.8
16	La Pr Sr CuO 1.65 0.2 0.15 4	32
17	La Nd Sr CuO 1.65 0.2 0.15 4	27
18	La Sm Sr CuO 1.65 0.2 0.15 4	10
19	La Eu Sr CuO 1.65 0.2 0.15 4	4.2
20	La Sr CuO 1.8 0.2 4	39
21	La Pr Sr CuO 1.6 0.2 0.2 4	33
22	La Nd Sr CuO 1.6 0.2 0.2 4	29
23	La Sm Sr CuO 1.6 0.2 0.2 4	23
24	La Eu Sr CuO 1.6 0.2 0.2 4	21
25	La Gd Sr CuO 1.6 0.2 0.2 4	18
26	La Pr Sr CuO 1.7 0.1 0.2 4	23
27	La Eu Sr CuO 1.7 0.1 0.2 4	17
28	La Gd Sr CuO 1.65 0.1 0.25 4	5

N	Composition, C.N.= 9	T_c, K
29	La Gd Sr CuO 1.75 0.15 0.1 4	0
30	La Pr Sr CuO 1.65 0.15 0.2 4	26
31	La Nd Sr CuO 1.65 0.15 0.2 4	23
32	La Sm Sr CuO	18
33	La Eu Sr CuO 1.65 0.15 0.2 4	15.2
34	La Gd Sr CuO 1.65 0.15 0.2 4	14
35	La Pr Sr CuO 1.6 0.15 0.25 4	4.2
36	La Nd Sr CuO 1.6 0.15 0.25 4	5
37	La Eu Sr CuO 1.6 0.15 0.25 4	6
38	La Gd Sr CuO 1.7 0.2 0.1 4	0
39	La Pr Sr CuO 1.55 0.2 0.25 4	0
40	La Nd Sr CuO 1.55 0.2 0.25 4	0
41	La Sm Sr CuO 1.55 0.2 0.25 4	4.2
42	La Eu Sr CuO 1.55 0.2 0.25 4	4.2
43	La Pr Sr CuO 1.2 0.6 0.2 4	29.5
44	La Y Sr CuO 1.6 0.25 0.15 4	0

The coefficient of linear correlation equals 0.3040 for the degree of freedom f=42 and the confidence level alpha = 0.05. So T_c statistically correlate with the following properties of element Ln (Table 4.3.2):

Table 4.3.2
The component properties of phases with composition $(La,Ln,Sr)_2CuO_4$ most influencing on T_c

Property	The value of correlation coefficient
concentration of Sr	-0.4710
3-rd potential of ionization of Ln	-0.3124

Property	The value of correlation coefficient
isobaric thermal capacity of Ln	-0.3121
melting temperature of Ln	-0.3835
heat of melting of Ln	-0.4009
heat of boiling of Ln	0.3671
Debye temperature of Ln	-0.4928

The most influential parameter is the Debye temperature of doped component Ln: the increasing Ln Debye temperature the critical temperature of transition to superconducting state decreases. The influence of other parameters of Ln component - third potential of ionization, isobaric standard thermal capacity, temperature and heat of melting, Sr concentration - is just the same.

4.4. T'-phases of $(Ln^{3+},M^{4+})_2CuO_4$ (M^{4+} = Ce^{4+} or Th^{4+}) composition

The sample for analysis included the data only about 8 T`-phases (Table 4.4.1). The coefficients of linear correlation of T_c with the following properties were calculated: concentration of Ln and M and all the properties of Ln component previously analysed.

Table 4.4.1
T'-Phases of composition $(Ln^{3+},M^{4+})_2CuO_4$

N	Composition, C.N.= 9	T_c, K
1	Nd Ce CuO 1.85 0.15 4	20
2	Nd Ce CuO 1.82 0.18 4	24
3	Nd Ce CuO 1.86 0.14 4	24
4	Pr Th CuO 1.85 0.15 4	19.5
5	Eu Ce CuO 1.85 0.15 4	8
6	Gd Ce CuO 0.195 1.005 4	0
7	Sm Th CuO 1.85 0.15 4	1.9
8	Gd Ce CuO 1.85 0.15 4	0

The critical value of coefficient of linear corelation equals 0.7067 for the degree of freedom f=6 and the confidence level alpha = 0.05. So T_c statistically correlate with the following properties of element Ln (Table 4.4.2):

Table 4.4.2
Ln component properties of T`-phases with composition $(Ln^{3+},M^{4+})_2CuO_4$ most influencing on T_c

Property	The value of correlation coefficient
3-rd potential of ionization of Ln	-0.8595
ionic radius of Ln	0.9108
number of electrons on the incomplete f-shell of Ln	-0.9005
standard entropy of individual substance for Ln	0.9522
isobaric thermal capacity of Ln	-0.7156
heat of boiling of Ln	0.8839

The major contribution in T_c of T`-phases brings the entropy of Ln: its increasing leads to the growth of T_c. The choice of dope of Ln with more high ionic radius, standard entropy of individual substance, and heat of boiling also favours the growth of T_c. On the opposite, T_c decreases with the growth of the third potential of ionization, the number of electrons on incomplete f-shell and isobaric standard thermal capacity of Ln^{3+} component.

4.5. T*-phases of $(Ln,Sr)(Ln`,Ln``)CuO_4$ (Ln, Ln` - La or Nd)

The sample for analysis included the data about 26 T*-phases (Table 4.5.1). The coefficients of linear correlation of T_c with the following properties were calculated: concentration of Ln and Sr (C.N.= 9) and Ln` and Ln`` (C.N. = 8) and also the properties of Ln`` component previously analysed for the component Ln.

Table 4.5.1
T*-Phases of composition $(Ln,Sr)(Ln',Ln'')CuO_4$

N	Composition	T_c, K
1	La Sm Sr CuO 0.84 0.96 0.2 4	21
2	La Eu Sr CuO 0.9 0.9 0.2 4	13.5
3	La Gd Sr CuO 0.9 0.9 0.2 4	13
4	LaTb Sr CuO 0.8 0.2 4	0
5	La Dy Sr CuO 1.08 0.72 0.2 4	0
6	La Ho Sr CuO 1.1 0.7 0.2 4	0

N	Composition	T_c, K
7	LaDy Sr CuO 0.8 0.2 4	0
8	LaGd Sr CuO 0.8 0.2 4	0
9	La EuSr CuO 0.8 0.2 4	0
10	La Eu Sr CuO 1.1 0.8 0.1 4	0
11	LaEu Sr CuO 0.9 0.1 4	0
12	La Eu Sr CuO 0.85 0.9 0.25 4	0
13	Nd Ce Sr CuO 1.33 0.27 0.4 4	19
14	Nd Ce Sr CuO 1.2 0.35 0.45 4	21.2
15	La Eu Sr CuO 0.95 0.9 0.15 4	0
16	La Eu Sr CuO 1.05 0.8 0.15 4	0
17	La Eu Sr CuO 1.15 0.7 0.15 4	0
18	Nd Ce Sr CuO 1.4 0.2 0.4 4	20
19	La Gd Sr CuO 1.1 0.8 0.1 4	0
20	La Sr Eu Ce CuO 0.75 0.25 0.85 0.15 4	0
21	La Sr GdCuO 0.75 0.25 4	0
22	La Sr Gd Ce CuO 0.75 0.25 0.9 0.1 4	0
23	Pr Ce Sr CuO 1.2 0.35 0.45 4	0
24	Pr Sm Sr CuO 1.4 0.25 0.35 4	0
25	Pr Ce Sr CuO 1.47 0.162 0.368 4	0
26	Pr Gd Sr CuO 1.4 0.25 0.35 4	0

The critical value of coefficient of linear correlation equals 0.3810 for the degree of freedom f=24 and the confidence level alpha = 0.05. So T_C statistically correlate with the following properties of element Ln`` (Table 4.5.2):

Table 4.5.2
The Ln`` component properties of T* - phases with composition (Ln, Sr) (Ln`, Ln``) CuO_4 most influencing on T_c

Property	The value of correlation coefficient
concentration of Ln	-0.4074
concentration of Sr	0.4074
ionic radius of Ln``	0.4023

Property	The value of correlation coefficient
number of electrons on the incomplete f-shell of Ln``	-0.3983

The major influence on T_c of T*-phases brings the concentration of Ln (Sr). The increasing of strontium concentration and corresponding decreasing of Ln concentration lead to the growth of T_c. The choice of Ln`` component with more high ionic radius, but small number of electrons in f-shell also favours the increase of T_c.

4.6. Brief discussion of the results

A small number of data about T-, T`-, T* - phases synthesized not so long ago did not let us to estimate the influence of oxygen concentration and the properties of all components, especially in more complicated phases. That's why during the further computer experiments it's advantageous to increase the analysed sample with new data in order to take these factors into consideration. The last is nesessary from the point of view that statistical estimations of samples containing less then 30-40 observations often do not allow to describe the real connections between properties.

The analysis of correlations can't explain the reason of important interdependences, their routs lie in the background of nature. That's why it's the work of experts - to analyse the cause and effect relations from the standpoint of physics and chemistry of HTSC.

It seems to be interesting to use the information about the component properties most influencing on T_c for the prediction of new HTSC and the estimation of their T_c with the help of artificial intellegence systems as it was performed during the search for the Chevrel phases [84,93].

CONCLUSIONS

1. The basic principles of prediction of inorganic compounds for new electro-optical, ferro-electric, superconducting, or semiconducting materials use computer learning strategies.

2. The ways for improvement of the reliability of the prediction are based on the utilization of databases for the selection of learning examples, expert assessment of data for computer learning, and comparison of predictions which have been obtained using various feature sets.

3. The classes of the inorganic compounds exhibiting the most promise for searching for new electro-optical, ferro-electric, superconducting, and semiconducting materials are determined on the basis of analysis of the application domains and the known data.

4. Results of predicting the crystal structure types (chalcopyrite, Th_3P_4, $CaFe_2O_4$, Yb_3S_4, Yb_3Se_4, $PbGa_2Se_4$, $NiCr_2Se_4$, spinel, or olivine) at normal pressure and room temperature for the compounds with composition of AB_2Se_4 are presented.

5. Analysis of predictions showed that the structures resembling olivine and $NiCr_2Se_4$ are an inherent feature of compounds with composition $A(IV)B(II)_2Se_4$, but the structure types Th_3P_4 and $NiCr_2Se_4$ are characteristic of compounds with composition $A(II)B(III)_2Se_4$.

6. Prediction of the crystal structure types (chalcopyrite, alfa- or beta-$NaFeO_2$, alfa-$LiFeO_2$, or TlSe) at standard conditions for compounds with composition ABX_2 was carried out. Analysis of the results shows also that the size of this learning set is too small for reliable prediction of new chalcopyrites of composition ABX_2.

7. The predictions of possibility of formation for the compounds with composition of A_3BCl_5 are presented. Analysis of results of prediction shows that few new compounds of the composition A_3BCl_5 form at normal pressure: In_3FeCl_5, Rb_3CoCl_5, and Tl_3CuCl_5.

8. Results of predicting the crystal structure types ($BaFeF_5$, $BaGaF_5$, $CaCrF_5$, $CaFeF_5$, or $SrFeF_5$) at normal pressure and room temperature for the compounds with composition of ABF_5 are presented. Analysis of predictions shows: the great number of new compounds with crystal structure type $BaFeF_5$ and $CaFeF_5$, which hold the promise for searching for new electro-optical materials, can be obtained.

9. Prediction of the crystal structure types at standard conditions for the compounds with composition A_2BF_6 were also carried out. For composition $A^I{}_2B^{IV}{}_6F$ types considered included: Na_2SiF_6, K_2PtCl_6, K_2GeF_6-II, K_2MnF_6-II, beta1-K_2UF_6, K_2ZrF_6, and trirutile. Analysis of results shows: the great number of predictions of new compounds with

crystal structure type K_2GeF_6-II and K_2ZrF_6 were obtained. New compounds with acentric space groups (crystal structure type Na_2SiF_6, space group P321): Na_2VF_6 and Na_2PaF_6, and (crystal type beta1-K_2UF_2, space group P6(-)2m): Cs_2TbF_6, Tl_2TbF_6, Cs_2NpF_6, Tl_2PuF_6, K_2AmF_6, Cs_2AmF_6, Cs_2CmF_6, Tl_2CmF_6, Rb_2BkF_6, Cs_2BkF_6, Tl_2BkF_6, Rb_2CfF_6, Cs_2CfF_6, and Tl_2CfF_6, which hold the promise for searching for new electro-optical materials, - were predicted also.

10. For composition $A^{II}{}_2B^{II}F_6$ types considered included: Ba_2MnF_6, Ba_2CuF_6, Pb_2ZnF_6, and rutile. Analysis of results shows: the great number of predictions of new compounds with acentric crystal structure type Ba_2MnF_6 were obtained, which hold the promise for searching for new electro-optical materials.

11. Prediction of the crystal structure types (calcite, aragonite, ilmenite, $NaClO_3$, $KBrO_3$, $LiNbO_3$, or perovskite) at standard conditions for the compounds with composition $A^IB^VO_3$ and $A^{II}B^{IV}O_3$ were also carried out. Analysis of results shows: few new lithium compounds with crystal structure type $LiNbO_3$, which hold the promise for searching for new electro-optical materials, were obtained.

12. Type of distortion (rhombic, hexagonal, monoclinic, or tetragonal) of ideal cubic perovskite cell at normal pressure and room temperature was predicted in addition. Analysis of results shows: the great number of predictions of new compounds with crystal structure type of cubic, rhombic and monoclinic perovskite, were obtained also for compounds of composition $A^{II}B^{IV}O_3$.

13. The search for statistical linear correlations between critical temperature of transition to superconducting state (T_c) and properties of high-temperature superconductors (HTSC) components was carried out. Complicated perovskite-like phases were analysed: phases "1-2-3", T-, T', and T*-phases. It has been suggested to use the information about the component properties most influencing on T_c will be used for the prediction of new HTSC and the estimation of their T_c with the help of artificial intellegence systems.

14. Successful solution of the goals to be sought is closely connected with the development of information-predicting system which was suggested by us [8,19-21].

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